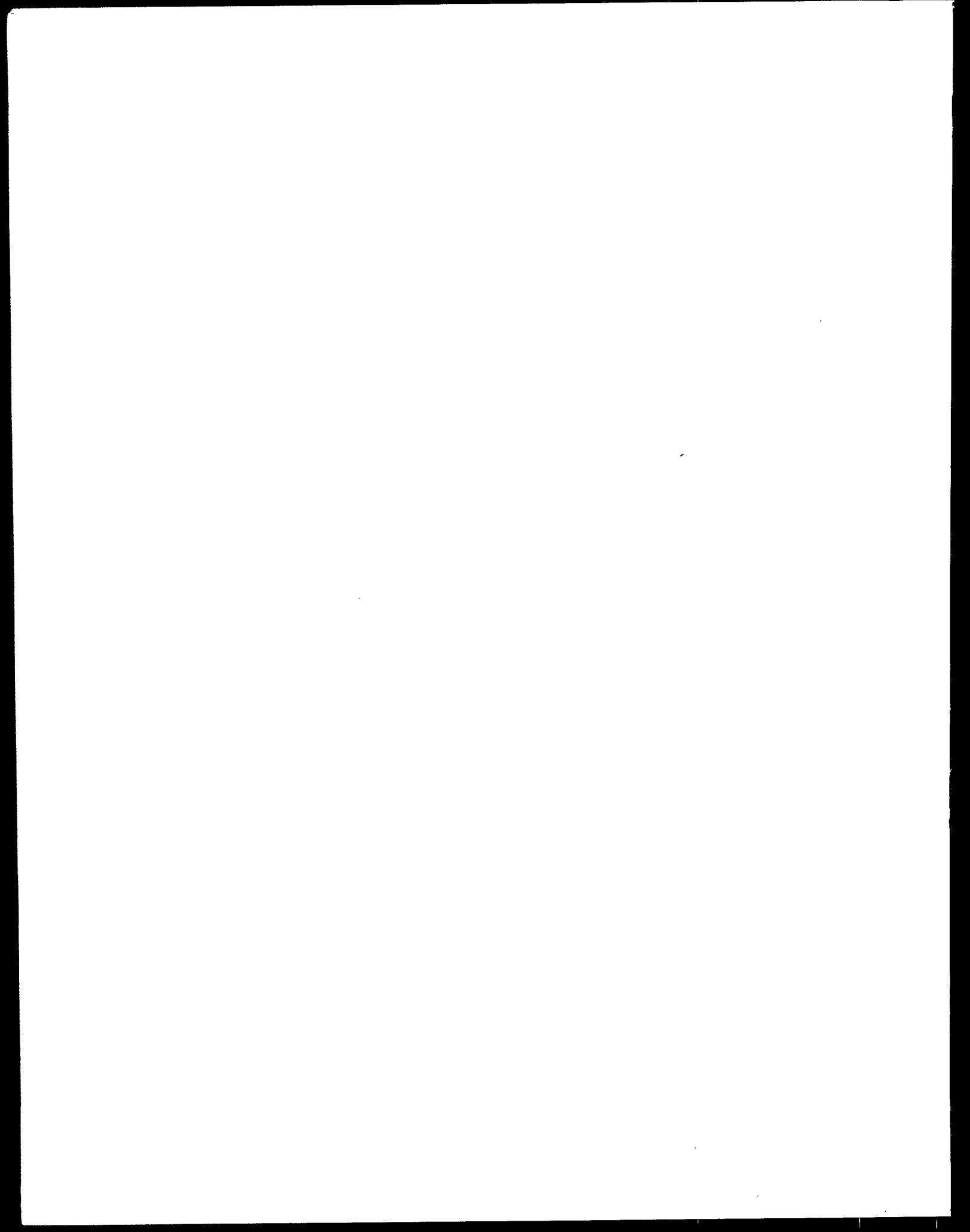**♻EPA**

Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities

Volume Two
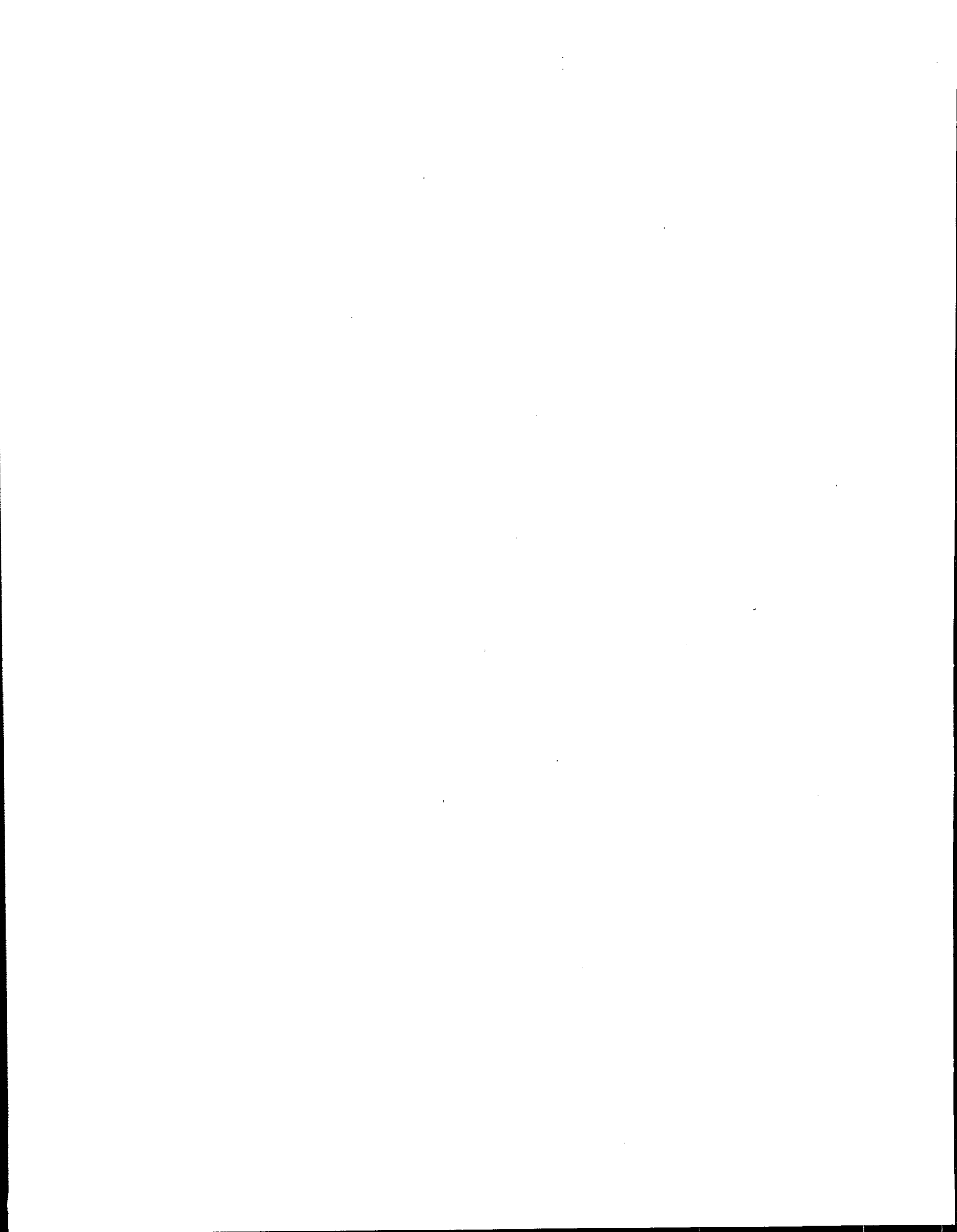## Appendix A

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APPENDIX A

CHEMICAL-SPECIFIC DATA

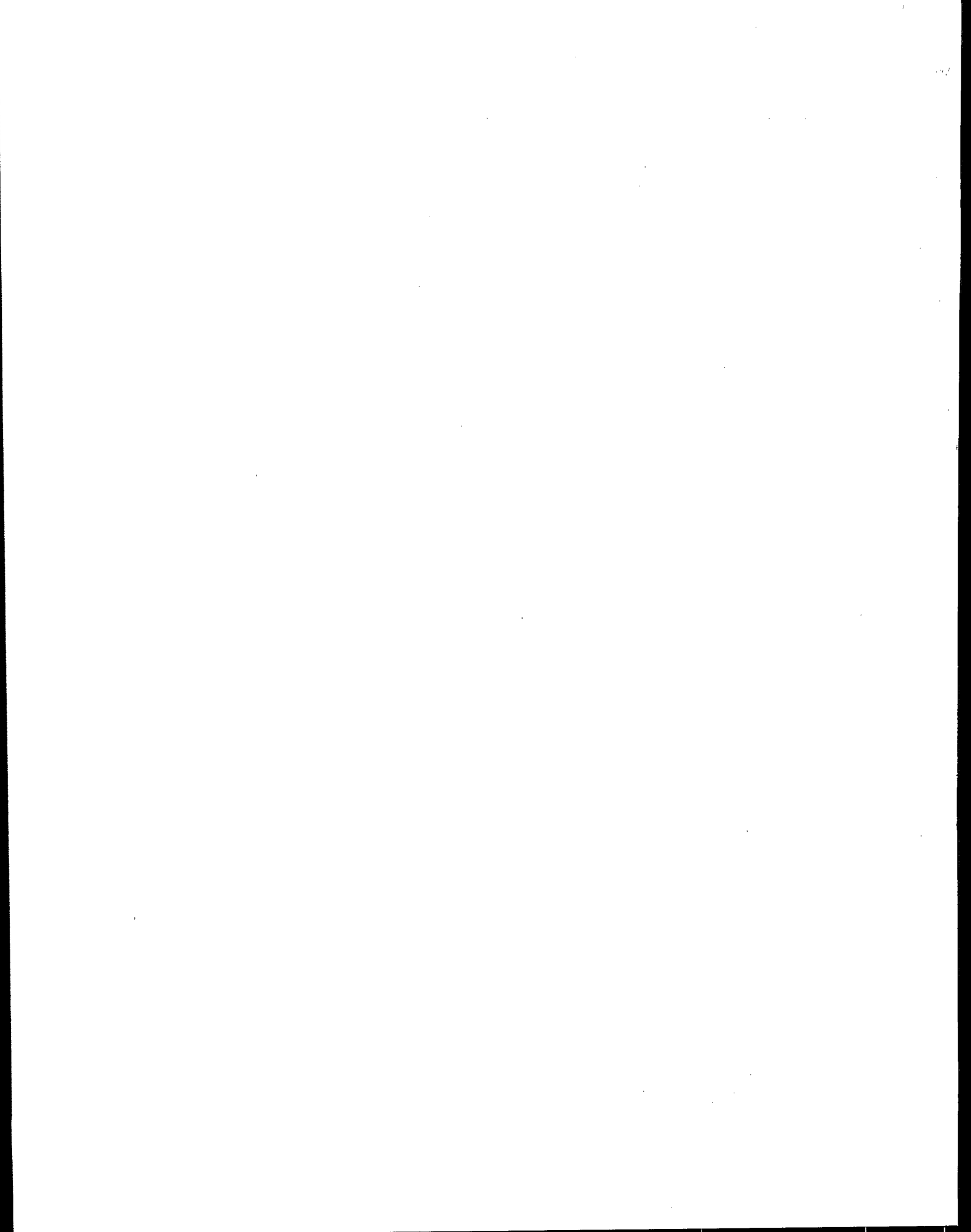### HUMAN HEALTH RISK ASSESSMENT PROTOCOL

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APPENDIX A-1

INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994c) for All HHRAs	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994)	PICs in Stack Emissions Actually Detected
50-00-0	Formaldehyde (methylene oxide)	K009, K010, K038, K040, K156, K157	X		X	X	
50-06-6	Phenobarbital						
50-07-7	Mitomycin						
50-18-0	Cyclophosphamide						
50-29-3	4,4'-DDT		X				
50-32-8	Benzo(a)pyrene	F032, F034, F037, F038, K001, K022, K035, K141, K142, K144, K145, K147, K148	X		X	X	X
50-55-5	Reserpine						
51-28-5	2,4-Dinitrophenol	K001	X			X	
51-43-4	Epinephrine						
51-52-5	Propylthiouracil						
51-79-6	Ethyl carbamate (urethane)					X	
52-85-7	Famphur						
53-70-3	Dibenzo(a,h)anthracene	F032, F034, K022, K141, K142, K144, K145, K147, K148	X			X	
53-96-3	2-Acetylaminofluorene						
54-11-5	Nicotine						
55-18-5	Nitrosodiethylamine						
55-38-9	Fenthion						
55-63-0	Nitroglycerine						
55-91-4	Diisopropylfluorophosphate (DFP)						
56-04-2	Methylthiouracil						
56-23-5	Carbon tetrachloride	F001, F024, F025, K016, K019, K020, K021, K073, K116, K150, K151, K157	X		X	X	X
56-38-2	Parathion						
56-49-5	3-Methylcholanthrene						
56-53-1	Diethylstilbestrol						
56-55-3	Benzo(a)anthracene	F032, F034, K001, K022, K035, K141, K142, K143, K144, K145, K147, K148	X		X	X	

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

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56-57-5	Nitroquinoline-1-oxide						
56-72-4	Coumaphos						
57-12-5	Cyanide		X				X
57-14-7	1,1-Dimethyl hydrazine	K107, K108, K109, K110					
57-24-9	Strychnine		X			X	
57-41-0	5,5-Diphenylhydantoin						
57-57-8	beta-Propiolactone						
57-74-9	Chlordane	K097	X			X	
57-97-6	7,12-Dimethylbenz(a)anthracene						
58-89-9	gamma-BHC (Lindane)						
58-89-9	Lindane (all isomers)					X	
58-90-2	2,3,4,6-Tetrachlorophenol	F020, F023, F027, F028, K001	X				
59-89-2	N-Nitrosomorpholine						
59-50-7	4-Chloro-3-methylphenol (p-chloro-m-cresol)	F004, K001					
60-09-3	Aminoazobenzene						
60-11-7	Dimethyl aminoazobenzene					X	
60-34-4	Methyl hydrazine						
60-35-5	Acetamide						
60-51-5	Dimethoate						
60-57-1	Dieldrin		X				
61-82-5	Amitrole						
62-38-4	Phenylmercury acetate						
62-44-2	Phenacetin						
62-50-0	Ethyl methanesulfonate		X			X	
62-53-3	Aniline	K083, K103, K104, K112, K113	X			X	
62-55-5	Thioacetamide						
62-56-6	Thiourea						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

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62-73-7	Dichlorovos		X				
62-74-8	Fluoroacetic acid, sodium salt						
62-75-9	N-Nitrosodimethylamine						
63-25-2	Carbaryl	K156					
64-17-5	Ethanol						
64-18-6	Formic acid (methanoic acid)	K009, K010	X			X	
64-64-7	Di-n-propylnitrosamine					X	
64-67-5	Diethyl sulfate						
65-85-0	Benzoic acid		X				X
66-27-3	Methyl methanesulfonate						
66-75-1	Uracil mustard						
67-56-1	Methanol		X				
67-64-1	Acetone		X				X
67-66-3	Chloroform (trichloromethane)	F024, F025, K009, K010, K019, K020, K021, K029, K073, K116, K149, K150, K151, K158	X		X	X	X
67-72-1	Hexachloroethane (perchloroethane)	F024, F025, K016, K030, K073	X		X	X	
68-12-2	Dimethyl formamide						
70-25-7	N-Methyl-N'-nitro-N-nitrosoguanidine (MNNG)						
70-30-4	Hexachlorophene		X			X	
71-43-2	Benzene	F005, F024, F025, F037, F038, K085, K104, K105, K141, K142, K143, K144, K145, K147, K151, K159	X		X	X	X
71-55-6	Methyl chloroform (1,1,1-trichloroethane)	F001, F002, F024, F025, K019, K020, K028, K029, K096			X	X	X
72-20-8	Endrin		X				
72-33-3	Mestranol						
72-43-5	Methoxychlor		X			X	
72-54-8	4,4'-DDD		X				
72-55-9	DDE		X			X	
72-57-1	Trypan blue						

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74-83-9	Bromomethane (methylbromide)	K131, K132	X		X	X	X
74-87-3	Chloromethane (methyl chloride)	F024, F025, K009, K010, K149, K150, K157	X		X	X	X
74-88-4	Methyl iodide (Iodomethane)						
74-90-8	Hydrogen cyanide	K011, K013					
74-93-1	Thiomethanol						
74-95-3	Methylene bromide		X		X	X	
74-97-5	Bromochloromethane				X	X	X
75-00-3	Chloroethane		X			X	
75-01-4	Vinyl chloride	F024, F025, K019, K020, K028, K029	X		X	X	X
75-05-8	Acetonitrile	K011, K013, K014	X		X		
75-07-0	Acetaldehyde		X			X	
75-09-2	Methylene chloride	F001, F002, F024, F025, K009, K010, K156, K157, K158	X			X	X
75-15-0	Carbon disulfide	F005	X		X	X	X
75-21-8	Ethylene oxide		X			X	
75-25-2	Bromoform		X			X	X
75-27-4	Bromodichloromethane		X		X	X	X
75-29-6	2-Chloropropane		X			X	
75-34-3	1,1-Dichloroethane	F024, F025	X		X	X	X
75-35-4	1,1-Dichloroethene	F024, F025, K019, K020, K029	X		X	X	
75-36-5	Acetyl chloride						
75-44-5	Phosgene (hydrogen phosphide)	K116				X	
75-45-6	Chlorodifluoromethane		X				X
75-55-8	1,2-Propylenimine (2-methyl aziridine)						
75-56-9	Propylene oxide						
75-60-5	Cacodylic acid						
75-69-4	Trichlorofluoromethane (Freon 11)	F001, F002	X			X	X
75-70-7	Trichloromethanethiol						

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75-71-8	Dichlorodifluoromethane		X			X	
75-86-5	2-Methylactonitrile						
75-87-6	Chloral						
76-01-7	Pentachloroethane	F024, F025					X
76-13-1	1,1,2-Trichloro-1,2,2-trifluoroethane(Freon 113)	F001, F002	X			X	X
76-44-8	Heptachlor	K097	X			X	
77-47-4	Hexachlorocyclopentadiene	F024, F025, K032, K033, K034	X			X	X
77-78-1	Dimethyl sulfate	K131				X	
78-00-2	Tetraethyl lead						
78-32-0	Tri-p-tolyl phosphate						
78-34-2	Dioxathion						
78-59-1	Isophorone		X				
78-83-1	Isobutyl alcohol	F005					
78-87-5	1,2-Dichloropropane		X			X	X
78-93-3	2-Butanone (methyl ethyl ketone)	F005	X		X	X	X
78-97-7	2-Hydroxypropionitrile						
79-00-5	1,1,2-Trichloroethane	F002, F024, F025, K019, K020, K095, K096	X		X	X	X
79-01-6	Trichloroethene	F001, F002, F024, F025, K018, K019, K020	X		X	X	X
79-06-1	Acrylamide	K014					
79-10-7	Acrylic acid						
79-11-8	Chloroacetic acid						
79-19-6	Thiosemicarbazide						
79-20-9	Methyl acetate		X				
79-22-1	Methyl chlorocarbonate						
79-34-5	1,1,2,2-Tetrachloroethane	F024, F025, K019, K020, K030, K073, K095, K150	X		X	X	
79-44-7	Dimethyl carbamoyl chloride						
79-46-9	2-Nitropropane	F005					

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80-62-6	Methyl methacrylate						
81-07-2	Saccharin						
81-81-2	Warfarin						
82-68-8	Pentachloronitrobenzene (PCNB)		X			X	
83-32-9	Acenaphthene	K022	X			X	X
84-66-2	Diethyl phthalate		X			X	X
84-74-2	Dibutyl phthalate		X		X	X	X
85-01-8	Phenanthrene	K022				X	X
85-44-9	Phthalic anhydride (1,2-benzenedicarboxylic anhydride)	K023, K024, K093, K094	X			X	
85-68-7	Butylbenzyl phthalate		X		X	X	X
86-30-6	N-Nitrosodiphenylamine		X				
86-50-0	Azinphos-methyl						
86-73-7	Fluorene	K022	X		X	X	X
86-88-4	alpha-Naphthylthiourea						
87-65-0	2,6-Dichlorophenol	K043					
87-68-3	Hexachlorobutadiene (perchlorobutadiene)	F024, F025, K016, K018, K030	X		X	X	X
87-86-5	Pentachlorophenol	F021, F027, F028, F032, K001	X		X	X	X
88-06-2	2,4,6-Trichlorophenol	F020, F023, F027, F028, K001, K043, K099, K105	X		X	X	X
88-74-4	o-Nitroaniline (2-nitroaniline)				X	X	X
88-75-5	2-Nitrophenol					X	X
88-85-7	Dinoseb						
90-04-0	o-Anisidine					X	
90-13-1	1-Chloronaphthalene						
91-20-3	Naphthalene	F024, F025, F034, K001, K022, K035, K060, K087, K145	X		X	X	X
91-22-5	Quinoline		X		X	X	X
91-57-6	2-Methylnaphthalene					X	
91-58-7	2-Chloronaphthalene		X			X	X

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91-59-8	2-Naphthylamine (beta-naphthylamine)						
91-80-5	Methapyrilene						
91-94-1	3,3'-Dichlorobenzidine		X			X	
92-52-4	Biphenyl		X		X	X	
92-67-1	4-Aminobiphenyl						
92-87-5	Benzidine		X				
92-93-3	4-Nitrobiphenyl						
93-72-1	Silvex	F027					
94-58-6	Dihydrosaffrole						
94-59-7	Safrole (5-(2-Propenyl)-1,3-benzodioxole)		X			X	
94-75-7	2,4-D		X			X	
95-06-7	Sulfallate						
95-47-6	o-Xylene (dimethyl benzene)		X		X	X	X
95-48-7	o-Cresol	F004	X			X	
95-50-1	1,2-Dichlorobenzene	F002, F024, F025, K042, K085, K105	X		X	X	X
95-53-4	o-Toluidine	K112, K113, K114	X			X	
95-57-8	2-Chlorophenol	K001	X			X	X
95-79-4	5-Chloro-2-methylaniline						
95-80-7	2,4-Toluene diamine	K112, K113, K114, K115, K027					
95-83-0	4-Chloro-1,2-phenylenediamine						
95-94-3	1,2,4,5-Tetrachlorobenzene	K085, K149, K150, K151	X		X	X	X
95-95-4	2,4,5-Trichlorophenol	F020, F023, F027, F028, K001	X		X	X	
96-09-3	Styrene oxide						
96-12-8	1,2-Dibromo-3-chloropropane		X		X	X	
96-18-4	1,2,3-Trichloropropane		X			X	
96-23-1	1,3-Dichloro-2-propanol						
96-45-7	Ethylene thiourea	K123, K124, K125, K126	X			X	

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97-63-2	Ethyl methacrylate		X			X	
98-01-1	Furfural		X			X	
98-07-7	Benzotrichloride	K015, K149	X			X	
98-82-8	Cumene		X		X	X	X
98-83-9	Methyl styrene (mixed isomers)		X			X	
98-86-2	Acetophenone		X			X	X
98-87-3	Benzal chloride						
98-95-3	Nitrobenzene	F004, K083, K103, K104	X			X	
99-09-2	3-Nitroaniline						
99-35-4	1,3,5-Trinitrobenzene		X			X	
99-55-8	5-Nitro-o-toluidine						
99-59-2	5-Nitro-o-anisidine						
99-65-0	1,3-Dinitrobenzene	K025	X			X	
100-01-6	4-Nitroaniline (p-nitroaniline)						
100-02-7	4-Nitrophenol (p-nitrophenol)					X	
100-25-4	1,4-Dinitrobenzene (p-dinitrobenzene)		X			X	
100-41-4	Ethylbenzene		X		X	X	X
100-42-5	Styrene		X		X	X	
100-44-7	Benzyl chloride	K015, K085, K149	X		X	X	
100-51-6	Benzyl alcohol						
100-52-7	Benzaldehyde		X		X	X	X
100-75-4	N-Nitrosopiperidine						
101-05-3	Anilazine						
101-14-4	4,4'-Methylenebis (2-chloroaniline)						
101-27-9	Barban						
101-55-3	4-Bromophenyl phenyl ether						
101-61-1	4,4'-Methylenebis (N,N-dimethylaniline)						

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101-68-8	Methylene diphenyl diisocyanate (MDI)						
101-79-9	4,4-Methylenedianiline						
101-80-4	4,4'-Oxydianiline					X	
102-82-9	Tributylamine						
103-33-3	Azobenzene		X		X	X	
103-85-5	Phenylthiourea						
105-60-2	Caprolactam						
105-67-9	2,4-Dimethylphenol	K001	X				
106-42-3	p-Xylene (dimethyl benzene)				X	X	X
106-44-5	p-Cresol (4-methyl phenol)	F004	X			X	
106-46-7	1,4-Dichlorobenzene	F024, F025, K085, K105, K149, K150	X		X	X	X
106-47-8	p-Chloroaniline		X			X	
106-49-0	p-Toluidine	K112, K113, K114	X			X	
106-50-3	p-Phenylenediamine						
106-51-4	Quinone					X	
106-88-7	1,2-Epoxybutane						
106-89-8	Epichlorohydrin (1-chloro-2,3 epoxypropane)	K017	X			X	
106-93-4	Ethylene dibromide	K117, K118, K136	X			X	
106-99-0	1,3-Butadiene				X	X	
107-02-8	Acrolein		X			X	
107-05-1	Allyl chloride	F024, F025					
107-06-2	1,2-Dichloroethane (ethylene dichloride)	F024, F025, K018, K019, K020, K029, K030, K096	X		X	X	X
107-07-3	2-Chloroethanol						
107-10-8	n-Propylamine						
107-12-0	Propionitrile						
107-13-1	Acrylonitrile	K011, K013	X		X	X	
107-18-6	Allyl alcohol						

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107-19-7	Propargyl alcohol		X			X	
107-20-0	Chloroacetaldehyde	K010					
107-21-1	Ethylene glycol (1,2-ethanediol)		X			X	
107-30-2	Chloromethyl methyl ether						
107-49-3	Tetraethyl pyrophosphate						
107-98-2	Propylene glycol monomethyl ether		X				
108-05-4	Vinyl acetate		X			X	
108-10-1	Methyl isobutyl ketone		X			X	X
108-18-9	Diisopropylamine						
108-31-6	Maleic anhydride	K023, K093	X			X	X
108-38-3	m-Xylene (dimethyl benzene)		X		X	X	X
108-39-4	m-Cresol	F004	X			X	X
108-46-3	Resorcinol					X	
108-60-1	bis (2-Chlorisopropyl)ether		X			X	X
108-67-8	1,3,5-Trimethylbenzene						X
108-87-2	Methylcyclohexane		X			X	X
108-88-3	Toluene	F005, F024, F025, K015, K036, K037, K149, K151	X		X	X	X
108-90-7	Chlorobenzene	F002, F024, F025, K015, K105, K149	X		X	X	X
108-95-2	Phenol	K001, K022, K087	X		X	X	X
108-98-5	Thiophenol (benzenethiol)						
109-06-8	2-Picoline	K026					
109-77-3	Malononitrile		X			X	X
109-88-4	2-Methoxyethanol		X			X	
109-89-7	Diethylamine						
109-99-9	Tetrahydrofuran		X				X
110-54-3	n-Hexane						X
110-75-8	2-Chloroethylvinyl ether		X			X	

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110-80-5	Ethylene glycol monoethyl ether	F005	X		X	X	
110-86-1	Pyridine	F005, K026, K157	X		X	X	
111-15-9	Ethylene glycol monoethyl ether acetate					X	
111-42-2	Diethanolamine						
111-44-4	bis(2-chloroethyl)ether	K017	X		X	X	
111-54-6	Ethylene(bis)dithiocarbamic acid						
111-76-2	Ethylene glycol monobutyl ether					X	
111-91-1	bis(2-chloroethoxy)methane				X	X	
114-26-1	Propoxur (Baygon)						
115-02-6	Azaserine						
115-29-7	Endosulfan		X				
115-90-2	Fensulfothion						
116-06-3	Aldicarb						
117-79-3	2-Aminoanthraquinone						
117-80-6	Dichlone						
117-81-7	bis(2-ethylhexyl)phthalate		X		X	X	X
117-84-0	Di-n-octylphthalate		X			X	
118-74-1	Hexachlorobenzene (perchlorobenzene)	F024, F025, K016, K018, K030, K042, K085, K149, K150, K151	X		X	X	X
118-96-7	2,4,6-Trinitrotoluene		X				
119-90-4	3,3'-Dimethoxybenzidine		X			X	
119-93-7	3,3'-Dimethylbenzidine						
120-12-7	Anthracene	K022	X		X	X	
120-58-1	Isosafrole						
120-62-7	Piperonyl sulfoxide						
120-71-8	p-Cresidine						
120-80-9	Catechol						
120-82-1	1,2,4-Trichlorobenzene	F024, F025, K085, K150	X		X	X	X

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994c) for All HHRAs	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994)	PICs in Stack Emissions Actually Detected
120-83-2	2,4-Dichlorophenol	K043, K099	X			X	
121-14-2	2,4-Dinitrotoluene	K025, K111	X			X	
121-44-8	Triethylamine	K156, K157					
121-69-7	N,N-Diethyl aniline						
121-75-5	Malathion		X				
122-09-8	a,a-Dimethylphenethylamine						
122-39-4	Diphenylamine	K083, K104	X			X	
122-66-7	1,2-Diphenylhydrazine		X			X	
123-31-9	Hydroquinone						
123-33-1	Maleic hydrazide		X			X	
123-38-6	Propionaldehyde					X	
123-63-7	Paraldehyde	K009, K010, K026					
123-91-1	Dioxane (1,4-dioxane)		X		X	X	X
124-48-1	Chlorodibromomethane		X				X
126-68-1	0,0,0-Triethyl phosphorothioate						
126-72-7	tris(2,3-dibromopropyl) phosphate						
126-75-0	Demeton-S						
126-98-7	Methacrylonitrile		X			X	
126-99-8	Chloroprene						
127-18-4	Tetrachloroethene (Perchloroethylene)	F001, F002, F024, F025, K016, K019, K020, K073, K116, K150, K151	X	X	X	X	X
129-00-0	Pyrene	K022	X		X		X
130-15-4	1,4-Naphthoquinone	K024					
131-11-3	Dimethyl Phthalate		X		X	X	
131-89-5	2-Cyclohexyl-4,6-dinitro-phenol		X			X	
131-89-5	2-Cycloyhexyl-4,6-dinitrophenol						
132-32-1	3-Amino-9-ethylcarbazole					X	
132-64-9	Dibenzofuran				X		

Note: See Table A-1 References and Discussion (Appendix A-4) for explanation of the information presented.

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CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994c) for All HHRAs	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994)	PICs in Stack Emissions Actually Detected
133-06-2	Captan						
133-90-4	Chloramben		X				
134-32-7	1-Naphthylamine (alpha-naphthylamine)						
137-17-7	2,4,5-Trimethylaniline						
137-26-8	Thiram						
140-57-8	Aramite						
140-88-5	Ethyl acrylate						
141-66-2	Dicrotophos						
143-33-9	Sodium cyanide	F007, F008, F009, F010, F011					
143-50-0	Kepone						
145-73-3	Endothall						
148-82-3	Melphalan					X	
151-50-8	Potassium cyanide	F007, F008, F009, F010, F011					
151-56-4	Ethylene imine (Aziridine)						
152-16-9	Octamethyl pyrophosphoramide						
156-60-5	(trans)1,2-dichloroethene	F024, F025	X			X	
156-62-7	Calcium cyanamide						
189-55-9	Dibenzo(a,i)pyrene						
191-24-2	Benzo(g,h,i)perylene	K022			X	X	
192-65-4	Dibenzo(a,e)pyrene						
192-97-2	Benzo(e)pyrene	K022				X	
193-39-5	Indeno(1,2,3-cd)pyrene	F032, F034, K001, K022, K035, K141, K142, K147, K148	X			X	
205-82-3	Benzo(j)fluoranthene	K022			X	X	
205-99-2	Benzo(b)fluoranthene (3,4-Benzofluoranthene)	K001, K022, K035, K141, K142, K143, K144, K147, K148	X			X	
206-44-0	Fluoranthene	K001, K022, K035	X		X	X	
207-08-9	Benzo(k)fluoranthene	F034, K022, K141, K142, K143, K144, K147, K148	X		X	X	
208-96-8	Acenaphthalene	K001, K022, K035	X		X	X	X

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994c) for All HHRAs	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994)	PICs in Stack Emissions Actually Detected
218-01-9	Chrysene	F037, F038, K001, K022, K035	X		X	X	
224-42-0	Dibenz(a,j)acridine						
225-51-4	Benz[c]acridine						
297-97-2	O,O-Diethyl O-pyrazinyl phosphorothioate						
297-97-2	Thionazine						
298-00-0	Methyl parathion		X				
298-02-2	Phorate	K038, K040	X				
298-03-3	Demeton-O		X				
298-04-4	Disulfoton		X				
299-84-3	Ronnel		X				
300-76-5	Naled		X				
302-01-2	Hydrazine						
302-17-0	Chloral hydrate						
303-34-1	Lasiocarpine						
305-03-3	Chlorambucil						
309-00-2	Aldrin		X				
311-45-5	Diethyl-p-nitrophenyl phosphate						
315-18-4	Mexacarbate						
319-84-6	alpha-Hexachlorocyclohexane (alpha-BHC)	F024	X			X	
319-85-7	beta-Hexachlorocyclohexane (beta-BHC)		X			X	
319-86-8	delta-BHC						
321-60-8	2-Fluorobiphenyl						
334-88-3	Diazomethane						
353-50-4	Carbon oxyfluoride						
357-57-3	Brucine						
367-12-4	2-Fluorophenol						
460-00-4	4-Bromofluorobenzene						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994c) for All HHRAs	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994)	PICs in Stack Emissions Actually Detected
460-19-5	Cyanogen (oxalonitrile)		X			X	
463-58-1	Carbonyl sulfide						
465-73-6	Isodrin						
470-90-6	Chlorfenvinphos						
479-45-8	Tetryl						
492-80-8	Auramine						
494-03-1	Chlornaphazin						
504-24-5	4-Aminopyridine						
505-60-2	Mustard gas						
506-61-6	Potassium silver cyanide	F006, F007, F008, F009, F010, F011, F012, F019, K007, K088					
506-64-9	Silver cyanide	F006, F012, F019, K007, K088					
506-68-3	Cyanogen bromide (bromocyanide)		X			X	
506-77-4	Cyanogen chloride		X			X	
510-15-6	Chlorobenzilate		X			X	
512-56-1	Trimethyl phosphate						
528-29-0	1,2-Dinitrobenzene (o-Dinitrobenzene)		X			X	
532-27-4	2-Chloroacetophenone					X	
534-52-1	4,6-Dinitro-o-cresol	F004				X	
540-36-3	1,4-Difluorobenzene						
540-73-8	1,2-Dimethylhydrazine					X	
540-84-1	2,2,4-Trimethylpentane					X	
541-53-7	Dithiobiuret						
541-73-1	1,3-Dichlorobenzene	F024, F025, K085, K105				X	X
542-62-1	Barium cyanide						
542-75-6	1,3-Dichloropropene		X			X	
542-76-7	3-Chloropropionitrile						
542-88-1	bis(Chloromethyl)ether	K017	X		X	X	

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994c) for All HHRAs	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994)	PICs in Stack Emissions Actually Detected
544-92-3	Copper cyanide						
557-19-7	Nickel cyanide						
557-21-1	Zinc cyanide						
563-12-2	Ethion						
563-68-8	Thallium(I)acetate						
584-84-9	2,4-Toluene diisocyanate	K027				X	
590-60-2	Bromoethene					X	
591-08-2	1-Acetyl-2-thiourea						
591-78-6	2-Hexanone (butyl methyl ketone)						
592-01-8	Calcium cyanide						
593-60-2	Vinyl bromide						
598-31-2	Bromoacetone						
602-87-9	5-Nitroacenaphthene						
606-20-2	2,6-Dinitrotoluene		X			X	
608-93-5	Pentachlorobenzene	F024, F025, K085, K149, K150, K151	X		X	X	X
615-53-2	N-Nitroso-N-methylurethane						
621-64-7	N-Nitroso-di-n-propylamine		X				
623-40-5	Toluene-2,6-diamine		X			X	
624-83-9	Methyl isocyanate					X	
628-86-4	Mercury fulminate						
630-10-4	Selenourea						
630-20-6	1,1,1,2-Tetrachloroethane	F024, F025, K019, K020, K030, K095	X		X	X	
636-21-5	o-Toluidine hydrochloride						
640-19-7	Fluoroacetamide						
680-31-9	Hexamethylphosphoramide						
684-93-5	N-Nitroso-N-methylurea						
692-42-2	Diethylarsine						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994c) for All HHRAs	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994)	PICs in Stack Emissions Actually Detected
696-28-6	Dichlorophenylarsine						
732-11-6	Phosmet						
755-04-5	Titanium tetrachloride						
757-58-4	Hexaethyl tetraphosphate						
759-73-9	N-Nitroso-N-ethylurea						
764-41-0	1,4-Dichloro-2-butene					X	
765-34-4	Glycidylaldehyde		X			X	
786-19-6	Carbophenothion						
822-06-0	Hexamethylene-1,5-diisocyanate					X	
924-16-3	N-Nitroso-di-n-Buetylamine		X			X	
930-55-2	N-Nitrosopyrrolidine						
959-98-8	Endosulfan I						
961-11-5	Tetrachlorvinphos						
1024-57-3	Heptachlor epoxide		X				
1031-07-8	Endosulfan sulfate						
1116-54-7	N-Nitrosodiethanolamine						
1120-71-4	1,3-Propane sultone					X	
1303-28-2	Arsenic pentoxide						
1314-32-5	Thallic oxide						
1314-62-1	Vanadium pentoxide						
1319-77-3	Cresols/cresylic acid (isomers and mixtures)	F004					
1327-53-3	Arsenic trioxide						
1330-20-7	Xylene (total)		X		X		X
1332-21-4	Asbestos						
1335-32-6	Lead subacetate						
1336-36-3	Polychlorinated biphenyls (209 congeners)		X		X	X	X
1338-23-4	2-Butanone peroxide						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994c) for All HHRAs	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994)	PICs in Stack Emissions Actually Detected
1464-53-5	1,2,3,4-Diepoxybutane						
1563-66-2	Carbofuran	K156, K158					
1582-09-8	Trifluralin						
1615-80-1	N,N'-Diethylhydrazine						
1634-04-4	Methyl tert butyl ether				X		
1718-51-0	Terphenyl-d14						
1746-01-6	2,3,7,8-Tetrachlorodibenzo(p)dioxin (TCDD)	F020, F022, F023, F026, F027, F028, F032	X		X	X	X
1836-75-5	Nitrofen						
1888-71-7	Hexachloropropene						
2037-26-5	Toluene-d8						
2104-64-5	EPN						
2303-16-4	Diallate (cis or trans)						
2310-17-0	Phosalone						
2385-85-5	Mirex						
2425-06-1	Captafol						
2763-96-4	5-(Aminomethyl)-3-isoxazolol						
2921-88-5	Chlorpyrifos		X				
3114-55-4	Chlorobenzene-d5						
3288-58-2	O,O-Diethyl S-methyl dithiophosphate						
3689-24-5	Tetraethyl dithiopyrophosphate						
4170-30-3	Crotonaldehyde (Propylene aldehyde)		X			X	
4549-40-0	N-Nitrosomethylvinylamine						
5131-60-2	4-Chloro-1,3-phenylenediamine						
5344-82-1	1-(o-Chlorophenyl)thiourea						
6533-73-9	Thallium(I)carbonate						
6923-22-4	Monocrotophos						
6959-48-4	3-(Chloromethyl)pyridine hydrochloride						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

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7005-72-3	4-Chlorophenyl phenyl ether	F020, F023, F027, F028					
7421-93-4	Endrin aldehyde						
7439-92-1	Lead	F035, F037, F038, K002, K003, K005, K046, K048, K049, K051, K052, K061, K062, K064, K069, K086, K100	X		X		X
7439-96-5	Manganese				X		X
7439-97-6	Mercury	K071, K106	X		X		X
7440-02-0	Nickel	F006	X		X	X	X
7440-22-4	Silver		X		X	X	
7440-28-0	Thallium		X		X	X	
7440-36-0	Antimony	K021, K161	X		X	X	X
7440-38-2	Arsenic	F032, F034, F035, K031, K060, K084, K101, K102, K161	X		X	X	X
7440-39-3	Barium		X		X	X	
7440-41-7	Beryllium		X		X	X	X
7440-43-9	Cadmium	F006, K061, K064, K069, K100	X		X	X	X
7440-47-3	Chromium (total)	F032, F034, F035, F037, F038, K090			X	X	X
7440-48-4	Cobalt					X	X
7440-50-8	Copper					X	X
7440-62-2	Vanadium						
7440-66-6	Zinc				X		X
7446-18-6	Thallium(I)sulfate						
7487-94-7	Mercuric chloride		X				X
7488-56-4	Selenium sulfide						
7647-01-0	Hydrogen Chloride (hydrochloric acid)		X			X	X
7664-38-2	Phosphoric acid						
7664-39-3	Hydrogen fluoride						
7664-41-7	Ammonia		X			X	X
7700-17-6	Crotoxyphos					X	X
7723-14-0	Phosphorus						

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7778-39-4	Arsenic acid						
7782-41-4	Fluorine						
7782-49-2	Selenium		X		X	X	
7782-50-5	Chlorine		X				
7783-00-8	Selenium dioxide						
7783-06-4	Hydrogen sulfide						
7786-34-7	Mevinphos						
7791-12-0	Thallium(I)chloride						
7803-51-2	Phosphine						
7803-55-6	Ammonium vanadate						
8001-35-2	Toxaphene (chlorinated camphene)	K041, K098					
8065-48-3	Demeton						
10102-43-9	Nitric oxide						
10102-44-0	Nitrogen dioxide						X
10102-45-1	Thallium(I)nitrate						
10595-95-6	N-Nitrosomethylethylamine						
11096-82-5	Arochlor-1260						
11097-69-1	Arochlor-1254		X				
11104-28-2	Arochlor-1221						
11141-16-5	Arochlor-1232						
12039-52-0	Thallium(I)selenite						
12672-29-6	Arochlor-1248						
12674-11-2	Arochlor-1016		X				
13071-79-9	Terbufos						
13171-21-6	Phosphamidon						
13463-39-3	Nickel carbonyl						
13765-19-0	Calcium chromate						

Note: See Table A-1 (References and Discussion (Appendix A-1) for explanation of the information presented.

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16752-77-5	Methomyl						
18540-29-9	Chromium (hexavalent)	F006, F019, K002, K003, K004, K005, K006, K007, K008, K048, K049, K050, K051, K061, K062, K069, K086, K100	X		X		X
18883-66-4	Streptozotocin						
19408-74-3	1,2,3,7,8,9-Hexachlorodibenzo(p)dioxin	F021, F022, F026, F027, F028, F032			X	X	
20816-12-0	Osmium tetroxide						
20830-81-3	Daunomycin						
20859-73-8	Aluminum phosphide						
21609-90-5	Leptophos						
22967-92-6	Methyl mercury		X		X	X	
23950-58-5	Pronamide		X			X	
25013-15-4	Methyl styrene		X				
25265-76-3	Phenylenediamine	K083, K103, K104					
25376-45-8	Toluenediamine						
26471-62-5	Toluene diisocyanate						
33213-65-9	Endosulfan II						
33245-39-5	Fluchloralin						
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzo(p)dioxin	F032			X	X	
39196-18-4	Thiofanox						
39227-28-6	1,2,3,4,7,8-Hexachlorodibenzo(p)dioxin	F021, F022, F026, F027, F028, F032			X	X	
39300-45-3	Dinocap						
40321-76-4	1,2,3,7,8-Pentachlorodibenzo(p)dioxin	F020, F021, F022, F023, F026, F027, F028, F032			X	X	X
53469-21-9	Arochlor-1242						
53494-70-5	Endrin ketone						
55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran	F032			X	X	
57117-41-6	2,3,4,7,8-Pentachlorodibenzofuran	F020, F021, F022, F023, F026, F027, F028, F032			X	X	X
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X	X	

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57653-85-7	1,2,3,6,7,8,-Hexachlorodibenzo(p)dioxin	F021, F022, F026, F027, F028, F032			X	X	
60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X	X	
67562-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	F032			X	X	
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X		
72918-21-9	1,2,3,7,8,9-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X	X	
109719-77-9	1,2,3,7,8-Pentachlorodibenzofuran	F020, F021, F022, F023, F026, F027, F028, F032			X	X	
125322-32-9	2,3,7,8-Tetrachlorodibenzofuran	F020, F022, F023, F026, F027, F028, F032			X	X	X
--	Beryllium compounds						
--	Cadmium compounds						
--	Chlorocyclopentadiene				X	X	
--	N-Chlorodiisopropyl amine						
--	N-Chloroisopropyl amine						
--	Chromium compounds						
--	Creosote	K001, K035					
--	Cyanide compounds	F006, F007, F008, F009, F010, F011, F012, F019, K007, K060, K088					
--	O-Decyl hydroxylamine						
--	Dibenzo(a,e)fluoranthene	K022			X	X	
--	Dibenzo(a,h)fluoranthene	K022			X	X	
--	Dibutylchloramine						
--	3,3-Dichloroisopropyl ether						
--	Dichloropentadiene					X	
--	Dimethylnitrosamine					X	
--	Lead compounds						
--	Nicotine salts						
--	2-Nitrodiphenylamine				X	X	
--	Octachlorodibenzo(p)dioxin				X	X	
--	Octachlorodibenzofuran				X	X	

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--	Phthalic acid esters						
--	Saccharin salts						
--	Sodium O-ethylmethylphosphonate Diisopropylamine						
--	Strychnine salts						
--	Thioamine						
--	O-decyl-hydroxylamine						
--	Acenaphthene-d10						
--	Antimony compounds						
--	Arsenic compounds (inorganic, including arsine)						
--	2-Chloro-1,3-butadiene	F024, F025					
--	Chrysene-d12						
--	Cobalt compounds						
--	Coke oven emissions						
--	Dibenz(a)anthracene	K001, K035					
--	1,4-Dichlorobenzene-d4						
--	Dichloroethylene	K073					
--	Dichloropropane	F024, F025					
--	Dichloropropanols	K017					
--	Dichloropropene	F024, F025					
--	Manganese compounds						
--	Mercury compounds						
--	Naphthalene-d8						
--	Nickel compounds						
--	Nitrobenzene-d5						
--	Perylene-d12						
--	Phenanthrene-d10						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994c) for All HHRAs	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994)	PICs in Stack Emissions Actually Detected
--	Phenol-d6						
--	Phenolic compounds	K060					
--	Phosphorodithioic and phosphorothioic acid esters	K036, K037, K038, K039, K040					
--	2,3,7,8-substituted Polychlorinated dibenzo(p)dioxin congeners (2,3,7,8-PCDDs)						
--	2,3,7,8-substituted Polychlorinated dibenzofuran congeners (2,3,7,8-PCDFs)						
--	Selenium compounds						
--	Tetrachlorobenzene	F024, F025					
--	2,4,6-Tribromophenol						
--	Trichloropropane	K017					

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

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APPENDIX A-1

COMPOUNDS OF POTENTIAL INTEREST

REFERENCES AND DISCUSSION

This discussion lists reference documents for each of the columns in Table A1-1 and briefly describes the quality of data associated with these references. The evaluation of chemical toxicity is also discussed at the end of this section. This information is presented for informational purposes only.

A1.1   COLUMN 1: CHEMICAL ABSTRACTS SERVICE (CAS) NUMBER

The CAS number is a unique number assigned to each compound in the table. Compounds are listed by CAS number, in ascending order, to prevent problems with alphabetization procedures or differences in common nomenclature.

A1.2   COLUMN 2: COMPOUND NAME

The most common compound name is listed. Where appropriate, common synonyms are also listed to aid the user in identifying particular compounds.

A1.3   COLUMN 3: COMPOUNDS LISTED IN 40 CFR PART 261 APPENDIX VII OR VIII

Appendix VII of Title 40 Code of Federal Regulations (40 CFR) Part 261 identifies compounds for which specific hazardous wastes, from specific and nonspecific sources, are listed (U.S. EPA 1995). Appendix VIII of 40 CFR Part 261 identifies acute hazardous wastes and toxic hazardous wastes associated with commercial chemical products, manufacturing chemical intermediates, and off-specification commercial chemical products (U.S. EPA 1995). This column lists hazardous waste codes for the associated compounds. This list is provided for reference purposes only, because it is commonly cited by other U.S. EPA combustion risk assessment documents as an original source of the product of incomplete combustion (PIC) lists. An explanation of the reasons for including a COPC on this list is beyond the scope of the HHRAP.

A1.4   COLUMN 4: CHEMICAL-SPECIFIC DATA AVAILABLE

This column lists those compounds for which the following are available (as presented in Appendix A-3): (1) chemical-specific physical and chemical information, and (2) chemical-specific fate-and-transport information.

A1.5   COLUMN 5: PICS RECOMMENDED BY U.S. EPA (1994a) FOR ALL HUMAN HEALTH RISK ASSESSMENTS (HHRA)

Compounds in this column marked with an "X" in the appropriate cells identified by U.S. EPA (1994a) as PICs to be included in all HHRAs. U.S. EPA (1994a) does not describe the basis or references for the inclusion of these PICs in all HHRAs. More information regarding these compounds is presented in Section 2.2 of the HHRAP.

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A1.6   COLUMN 6: PICS IDENTIFIED IN COMBUSTION UNIT EMISSIONS (U.S. EPA 1993)

Compounds in this column marked with an "X" in the appropriate cells are identified in U.S. EPA (1993) as PICs. The source documents for these tables cited by U.S. EPA (1993) are described in the following subsections. These references have been cited by this and other U.S. EPA reference documents as "sources" of information regarding PIC emissions from hazardous waste combustion units. This document—U.S. EPA (1993)—has, in turn, been cited by later guidance documents as a "source" of information regarding PIC emissions from hazardous waste combustion units. However, as is indicated by the listing of the references from Dempsey and Oppelt (1993) (which is a summary of existing information), many of the reference documents appear to simply cite additional "sources" of information. The original research and sampling data regarding PIC emissions have not yet been identified but, based on a preliminary review of the information below, the sources of the "original" information cited by all of the most common reference documents may be limited and may have been published over 15 years ago.

A1.6.1 Demsey and Oppelt (1993)

The sections of Demsey and Oppelt (1993) regarding PICs from hazardous waste combustion facilities ("Combustion Byproduct Emissions" and "Table XVII: Organics that Could Potentially be Emitted from Devices Burning Hazardous Waste") cite the following references:

- U.S. EPA (1989b) does not include a list of PICs from combustion sources. U.S. EPA (1989b) discussed ways of ensuring that PIC emissions do not pose an unacceptable risk to human health and the environment. Stack gas carbon monoxide (CO) concentration is a good indicator of combustion efficiency; therefore, controlling CO is a prudent and reasonable approach to minimizing the potential risk from PICs. The destruction and removal efficiency (DRE) standard of 40 CFR Part 264.242(a) limits stack emissions of principal organic hazardous constituents (POHC) to 0.01 percent (or 0.0001 percent for dioxin-containing waste) of the quantity of POHC in the waste. This standard, however, does not impose a limit on PICs. Therefore, a limit of 100 parts per million by volume (ppmv) (Tier I) was imposed, below which PIC emissions do not pose unacceptable risks to human health. The proposed rule allows a waiver to the 100-ppmv CO limit, by (1) restricting total hydrocarbon (THC) emissions to 20 ppmv (Tier II), or (2) showing that THC emissions do not pose an unacceptable health risk by using prescribed risk assessment procedures.

  The above limitations were also provided in the Federal Register, dated January 23, 1981 (U.S. EPA 1981) and April 27, 1990 (U.S. EPA 1990b)

- U.S. EPA (1981) does not contain any information regarding PICs not contained in U.S. EPA (1989b). There is no discussion of "risk" in this document. Although the notice deals with permitting standards, there is no risk-based approach, and it appears to be an entirely technical discussion. Specifically, it deals with updated material for specific parts of 40 CFR.

  - 40 CFR Part 122 (Incinerator Facility Permits)
  - 40 CFR Part 264 (General Standards for Hazardous Waste Incineration)

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- 40 CFR Part 265 (Interim Status Standards for Hazardous Waste Incineration)

Standards are technology-based, not risk-based.

- U.S. EPA (1990a) describes amendments to the hazardous waste incinerator regulations for the following purpose:

> Improve control of toxic metal emissions, HCl emissions, and residual organic emissions; amend the definitions of incinerators and industrial furnaces; propose definitions for plasma arc incinerators and infrared incinerators; propose to regulate carbon regeneration units as thermal treatment devices; and make a number of minor revisions to permitting procedures.

U.S. EPA (1990a) also states the following:

> The database on PIC emissions is limited therefore, the risk assessments may under-estimate risk. The assessments consider only the organic compounds that have been actually identified and quantified. Zero to 60 percent of total unburned hydrocarbon emissions have been chemically identified at any particular facility. Thus, the bulk of the hydrocarbon emissions have not been considered in those risk assessments. Although many of the unidentified, unquantified organic compounds may be non-toxic, some fraction of the organic emissions is undoubtedly toxic. . . .data on typical PIC emissions from hazardous waste combustion sources were compiled and assessed in recent EPA studies. These studies identified 37 individual compounds in the stack gas of the eight full-scale hazardous waste incinerators tested, out of which 17 were volatile compounds and 20 semivolatile compounds. Eight volatile compounds (benzene, toluene, chloroform, trichloroethylene, carbon tetrachloride, tetrachloroethylene, chlorobenzene, and methylene chloride), and one semivolatile compound (naphthalene) were identified most frequently in more than 50 percent of the tests. Some of these compounds are carcinogenic.

The sources for these statements appear to be Wallace and others (1986) and Trenholm and Lee (1986).

Trenolm and Lee (1986), prepared by Andrew R. Trenholm of Midwest Research Institute and C.C. Lee at the U.S. EPA Hazardous Waste Engineering Research Laboratory, discussed that emissions from incinerators are only characterized for constituents listed in Appendix VIII. However, constituents not listed in Appendix VIII are also emitted from the stacks.

Data was obtained from HWERL-sponsored tests at eight hazardous waste incinerators, nine boilers that co-fired hazardous wastes, and five mineral processing kilns that fired hazardous wastes as fuel. In addition, SVOC emissions data for two municipal solid waste incinerators and seven coal-fired power plants were also reviewed. The common PICs are presented in the following table:

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Volatile PICs Most Frequently Present in Stack Gases	
VOCs	**SVOCs**
Benzene	Naphthalene
Toluene	Phenol
Carbon Tetrachloride	Bis(2-ethylhexyl)phthalate
Chloroform	Diethylphthalate
Methylene Chloride	Butylbenzylphthalate
Trichloroethylene	Dibutylphathlate
Tetrachloroethylene	
1,1,1-Trichloroethane	
Chlorobenzene	

Tests were conducted for three incinerator runs to search for constituents not listed in Appendix VIII . These constituents include:

Non-Appendix VIII Constituents Present in Highest Concentrations in Stack Gases	
Acetone	Ethylbenzaldehyde
Ethylbenzene	Ethylbenzoic acid
Acetophenone	Ethylphenol
Benzaldehyde	Ethylphenyl-ethanone
Benzenedicarboxaldehyde	Ethynylbenzene
Benzoic acid	Phenylacetylene
Chlorocyclohexanol	1,1'-(1,4-phenylene)bisethanone
Cyclohexane	Phenylpropenol
Cyclohexanol	Propenylmethylbenzene
Cyclohexene	Tetramethyloxirane
Dioctyl adipate	Trimethylhexane
Ethenyl ethylbenzene	

Emission rates of compounds not in the waste feed were also provided.

- U.S. EPA (1985) does not include a list of PICs from combustion sources. U.S. EPA (1985) discussed views and reviews by the Environmental Effects, Transport, and Fate

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Committee of the Science Advisory Board of issues related to the environmental impacts of the incineration of liquid hazardous wastes at sea and on land. Several issues were addressed, including issues concerning the combustion and incineration of hazardous waste. Major findings of the committee were as follows:

- Fugitive emissions and spills may release as much or more material to the environment than the direct emissions from waste incineration processes.

- Numerous PICs are formed during combustion processes. However, only a fraction of them are identified or detected. It is possible that the aggregate of all compound emissions that are not categorized as other POHCs or PICs can be more toxic and pose greater risks than those listed. Although 99.99 percent DRE has been claimed, if the unburned or undetected hydrocarbon output is included, the DRE may actually be less than 99.99 percent. Therefore, the concept of destruction efficiency used by EPA was found to be incomplete and not useful for subsequent exposure assessments. All emissions and effluents must be identified and quantified, including their physical form and characteristics.

- Local site-specific conditions must be used in characterizing exposure to receptors from waste incinerator emissions.

- The evaluation of exposure durations and concentrations should be based on a detailed assessment of transport processes and the habits of the exposed organisms. The role of food chains needs particular attention.

- At a minimum, the toxicities of representative emissions and effluents from incinerators should be tested on sensitive life stages of representative aquatic and terrestrial vertebrates, invertebrates, and plants of ecological importance.

• U.S. EPA (1990b) does not include a list of PICs from combustion sources. It was prepared by the PIC subcommittee of the Science Advisory Board to review the OSW proposal to control emissions of PICs from hazardous waste incinerators by instituting process controls that are based on CO and THC emission concentrations. U.S. EPA risk assessments indicate that emissions of PICs at currently measured levels are not likely to produce human effects. However, because the current DRE standard applies only to designated POHCs, 99.99 percent DRE does not preclude the possibility that emission of PICs could present significant human health risk. The following summarizes the major findings of the subcommittee review.

- The concept of using CO and THC as guidance for incinerator operational control is reasonable.

- At low CO levels, CO correlates well with THC; therefore, limiting CO in order to ensure high combustion efficiency and low THC levels is reasonable. At high CO concentrations, CO and THC do not correlate well; therefore, relying solely on the controlling of CO may not provide a reasonable control for THC. Continuous emissions monitoring of THC is preferred. Quantification of PICs alone is not

practical with the sampling techniques that are available, primarily because PICs are normally emitted in the range of parts per billion (ppb) to parts per trillion (ppt).

- A 100-ppmv limit for CO is reasonable. However, supporting documentation does not demonstrate that a CO concentration of 100 ppmv is better than 50 ppmv or 150 ppmv.

- Continuous emissions monitoring of THC with a cold system appears to be practical for routine operations. However, a hot transfer line produces better analysis of THC concentrations and detection of a larger fraction of the THCs emitted.

- The database characterizing PICs in emissions would not allow a correlation to be established with CO or THC levels for various combustion devices and conditions. Limited data introduces large uncertainties into U.S. EPA's risk assessment. Therefore, U.S. EPA's site-specific risk assessment process is limited in its usefulness in establishing acceptable THC levels. However, the risk assessment procedures are risk-based.

- U.S. EPA (1987) is a report prepared by Andrew R. Trenholm, Acurex Corporation, California, and staff members from the U.S. EPA Hazardous Waste Engineering Research Laboratory in Cincinnati, Ohio. The paper discussed the lack of information on total emissions from combustion of hazardous wastes, particularly under conditions of less than optimal performance. The focus issue was whether additional constituents that are listed in Appendix VIII or not listed in Appendix VIII which were not identified in early tests might be emitted from hazardous waste combustion units. To address this issue and related issues, U.S. EPA initiated this project to qualitatively and quantitatively study the characteristics of all possible effluents, under steady-state and transient conditions. The following summarizes the major findings:

  - THC emissions detected as specific compounds ranged from 50 to 67 percent for five runs and were 91 percent for one run. The fraction of THC not detected is most likely explained by uncertainty in the measurements or other analytical problems.

  - Methane accounted for the largest fraction of THC.

  - Oxygenated aliphatic compounds made up the largest class of compounds among the SVOCs, both in total mass and number of compounds.

  - Transient upsets did not cause significant increases in the concentration of SVOCs or most VOCs. Three VOCs that were increased were methane, methylene chloride, and benzene.

  - Particulate and HCl emissions did not change between the steady-state and transient test runs.

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- Duval and Rubey (1976) was prepared by D.S. Duval and W.A. Rubey of the University of Dayton Research Institute, Ohio. The objective of the study was to provide data from which requirements can be assigned for the thermal disposal of kepone. This report was primarily concerned with the high-temperature destruction of kepone, with DDT and Mirex used as comparative Analog. Laboratory tests were conducted to establish destruction temperature characteristics of the vaporized pesticides at preselected residence times. The following summarizes the major findings.

  - Kepone was essentially destroyed at a 1-second residence time and a temperature range of 500°C to 700°C, depending on the pesticide.

  - Major decomposition products detected were hexachlorocyclopentadiene and hexachlorobenzene for both kepone and Mirex. These products were formed in different thermal regions.

  - The study demonstrated that the chemical nature of the effluent products depends on the temperature and residence time that the basic molecule experiences.

- Duval and Rubey (1977) discusses the experimental destruction temperature and residence time relationships for various PCB compounds and mixtures of PCBs. The document states that "upon thermal stressing in air, PCBs decomposes to low-molecular-weight products." However, the document does not identify any of these low-molecular-weight products. In fact, the document states directly that the products were not identified in the study. It further recommends that additional research be conducted on the "degradation products and effluents."

- Dellinger, Torres, Rubey, Hall, and Graham (1984) was prepared by Barry Dellinger and others of the University of Dayton, Ohio. This paper presented the gas-phase thermal stability method under controlled laboratory conditions to rank the incinerability of compounds. The objective of this study was to determine the gas-phase thermal decomposition properties of 20 hazardous organic compounds.

  The compounds were selected on the basis of (1) frequency of occurrence in hazardous waste samples, (2) apparent prevalence in stack effluents, and (3) representativeness of the spectrum of hazardous waste organic waste materials. The following summarizes the major findings.

  - Gas-phase thermal stability method is a more effective means of ranking the incinerability of hazardous compounds in a waste.

  - Numerous PICs were formed during the thermal decomposition of most of the compounds tested. However, PICs were not identified.

  - Destruction efficiency of 99.99 percent is achieved at 2 seconds mean residence time in flowing air at 600°C to 950°C.

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- No single physical or chemical property describes the ranking scheme for incinerability.

• Dellinger, Hall, Graham, Mazer, Rubey, and Malanchuk (1986) was prepared by Barry Dellinger, B. Douglas, L. Hall, John L. Graham, Sueann L. Mazer, and Wayne A. Rubey of the University of Dayton Research Institute, Dayton, Ohio, and Myron Malanchuk of U.S. EPA, Cincinnati, Ohio. The paper discussed the development of an incineration model based on laboratory studies conducted by using the nonflame mode of hazardous waste thermal decomposition. The results of these studies were compared to the flame-mode studies and field tests to evaluate the incineration model proposed. The model was based on the premise that incinerators do not operate continuously at optimum conditions. As a result, 1 percent or more of the feed and its flame treatment products must undergo further decomposition in the nonflame region to meet the DRE criterion of greater than 99.99 percent.

In the past, several methods were used to rank the incinerability of compounds. Nonflame studies, however, indicated that tests on compounds conducted at low oxygen concentrations provided a better correlation with field tests to determine the relative incinerability of compounds. Four experimental studies were conducted to develop and expand the database on POHCs and PICs.

Studies were conducted on individual compounds to evaluate degradation compounds and PICs from the original parent compound. The thermal degradation of 2,3',4,4',5-PCB was studied under four reaction atmospheres (at varying levels of oxygen) at a constant gas phase residence time of 2.0 seconds. Tests were conducted at temperatures ranging from 500°C to 1,000°C. Tests indicated that the yield of combustion products decreased with increased oxygen levels. Numerous major degradation products were identified from the thermal degradation of 2,3',4,4',5-PCB, including:

- Penta-, tetra-, and trichlorodibenzofurans
- Tetra- and trichlorobiphenyls
- Tri- and dichlorobenzene
- Tetra- and trichloronaphthalene
- Tri- and dichlorochlorophenylethlyene
- Tetrachlorobiphenylenes
- C_9H_8OCl
- $C_{10}H_3Cl_3$

Thermal decomposition of chloroform was studied. Numerous decomposition products were identified, including:

- CCl_4
- $C_2H_4Cl_2$
- C_2HCl_3
- C_2HCl_5
- C_2Cl_2
- C_2Cl_4

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- C_3Cl_4
- C_4Cl_6

Thermal decomposition of polychlorinated phenols was studied in nitrogen (N_2) and oxygen atmospheres because of the potential formation of polychlorinated dibenzodioxins. Pentachlorophenol (PCP) thermal decomposition was studied. Numerous decomposition products of PCP were identified in N_2 and/or air atmospheres, including:

- Dichlorobutadiyne (in N_2)
- Tetrachloroethylene (in air)
- Tetrachloropropyne (in air)
- Trichlorofuran (in air)
- Tetrachlorofuran (in air)
- Trichlorobenzene (in N_2 and air)
- Tetrachlorobenzene (in N_2 and air)
- Pentachlorobenzene (in N_2 and air)
- Hexachlorobenzene (in N_2)
- Octachlorostyrene (in N_2)
- Hexachlorodihydronaphthalene (in N_2 and air)

The paper concluded that PICs in the air atmosphere may have formed directly from the parent material, whereas, in the nitrogen atmosphere, the principal PICs may have evolved from the thermal decomposition of other PICs.

- Kramlich, Seeker, and Heap (1984) does not include a list of PICs from combustion sources. It was prepared by J.C. Kramlich, W.R. Seeker, and M.P. Heap of Energy and Environmental Research Corporation, California; and C.C. Lee of the Industrial Waste Combustion Group, U.S. EPA. This paper presented a research program to study the flame-mode incineration of hazardous waste liquids in laboratory scale reactors. The objective of this study was to supply the flame-mode data that will be used in evaluating the applicability of various approaches to ranking the ease of incinerability.

  Five compounds were tested—chloroform, 1,1-dichloroethane, benzene, acrylonitrile, and chlorobenzene—because (1) their range of incinerabilities is broad, and (2) they are representative of liquid hazardous wastes. The following summarizes the findings.

  - The flame section of the incinerator destroys greater than 99.995 percent of the wastes.

  - The post-flame region destroys the remainder of the wastes.

  - The destruction efficiency is reduced because of flame-related failures.

  - Incinerability ranking depends on actual failure condition.

  - No incinerability ranking system completely predicts the destruction efficiency of the compounds tested for all failure conditions.

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- Trenholm and Hathaway (1984) was prepared by Andrew Trenholm and Roger Hathaway of Midwest Research Institute (MRI) in Missouri, and Don Oberacker, U.S. EPA, Cincinnati, Ohio. PICs were defined as any Appendix VIII hazardous organic constituent detected in the stack gas but not present in the waste feed at a concentration of 100 micrograms per gram or higher. Benzene and chloroform were the most commonly found PICs. PIC emissions were comparable to POHC emissions in concentration and total mass output. This document discussed PIC formation mechanisms and criteria for PIC formations.

  MRI conducted a series of tests at eight operating hazardous waste incineration facilities and analyzed the collected samples for PICs. These tests were conducted as part of the technical support of U.S. EPA's preparation of a regulatory impact analysis for hazardous waste incinerators. Each incinerator had a liquid injection burner, and some facilities also included a rotary kiln or hearth. Three incinerators had no air pollution control devices. The remaining five had wet scrubbers for HCl control, and four of these had other particulate control devices. Twenty-nine compounds were classified as PICs from the eight incinerator tests and are presented in Table A1.6-1. In general, PIC concentrations were slightly higher than POHC concentrations, although this ratio varied from site to site. PIC output rate very rarely exceeded 0.01 percent of the POHC input rate. The document stated that the measurement of Appendix VIII compounds at low concentrations in the waste feed, auxiliary fuel, and inflow streams to control systems is often necessary to explain the presence of PICs.

- Olexsey, Huffman, and Evans (1985) was prepared by Robert A. Olexsey and others of the U.S. EPA Hazardous Waste Engineering Research Laboratory in Cincinnati, Ohio. This document discussed PIC generation mechanisms and criteria for PIC formations. The paper provided data on emissions of PICs during full-scale tests conducted on incinerators and boilers burning hazardous waste (Trenholm and others 1984; Castaldini and others 1984). The documents referenced by this paper summarized a series of full-scale tests conducted on seven incinerators and five boilers conducted by U.S. EPA to support its regulatory development for incinerators and boilers. Commonly found PICs identified in these tests are presented in Tables A1.6-2 and A1.6-3.

- For incinerators, ratios of PIC emissions to POHC input ranged from 0.00007 to 0.0028 percent; and ratios of PIC emissions to POHC emissions ranged from 0.01 to 3.89. For boilers, ratios of PIC emissions to POHC input ranged from 0.0032 to 0.3987 percent, and ratios of PIC emissions to POHC emissions ranged from 5.44 to 22.5. These data indicated that PIC emissions were higher for boilers than for incinerators; that is, PIC emissions were reduced with increased POHC DRE which is higher for incinerators. The document proposed seven methods to control PICs and recommended further research on PIC generation mechanisms and control technologies.
- Trenholm, Kapella, and Hinshaw (1992) was prepared by Andrew R. Trenholm and David W. Kapella of MRI in North Carolina and Gary D. Hinshaw of MRI in Missouri. The paper discusses the following issues regarding emissions from incinerators that burn hazardous waste: (1) emissions of specific constituents presented in Appendix VIII, (2) emissions of specific compounds or types of compounds, and (3) data on the size and

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molecular weight of compounds emitted. The following were among the major issues discussed.

- PICs were studied through U.S. EPA-sponsored tests at eight incinerators, nine industrial boilers, and five mineral processing kilns. The study was limited to compounds presented in Appendix VIII. In all, 52 organic compounds (32 VOCs and 20 SVOCs) were identified. The VOC concentrations were significantly higher than the SVOC concentrations. PICs listed in this paper included benzene, toluene, carbon tetrachloride, trichloromethane, dichloromethane, trichloroethene, tetrachloroethene, 1,1,1-trichloroethane, cholorobenzene, naphthalene, and phenol.

TABLE A1.6-1

PICS IDENTIFIED BY TRENHOLM AND HATHAWAY (1984)

PICs Found In Stack Effluents			
PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Benzene	6	12	670
Chloroform	5	1	1,330
Bromodichloromethane	4	3	32
Dibromochloromethane	4	1	12
Naphthalene	3	5	100
Bromoform	3	0.2	24
Chlorobenzene	3	1	10
Tetrachloroethylene	3	0.1	2.5
1,1,1,-Trichloroethane	3	0.1	1.5
Toluene	2	2	75
o-Nitrophenol	2	2	50
Methylene chloride	2	2	27
Phenol	2	4	22
2,4,6-Trichlorophenol	1	110	110
Carbon disulfide	1	32	32
o-Chlorophenol	1	22	22
2,4-Dimethylphenol	1	21	21
Methylene bromide	1	18	18
Bromochloromethane	1	14	14
Trichlorobenzene	1	7	7
Hexachlorobenzene	1	7	7

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PICs Found In Stack Effluents			
Diethyl phthalate	1	7	7
Pentachlorophenol	1	6	6
Dichlorobenzene	1	4	4
Chloromethane	1	3	3
Methyl ethyl ketone	1	3	3
Bromomethane	1	1	1
Pyrene	1	1	1
Fluoranthene	1	1	1

Notes:

    ng/L   =   Nanograms per liter
    PIC   =   Product of incomplete combustion

TABLE A1.6-2

VOLATILE PICS MOST FREQUENTLY IDENTIFIED IN BOILER EMISSIONS
(OLEXSY, HUFFMAN, AND EVANS 1985)

PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Chloroform	5	4.2	1,900
Tetrachloroethylene	5	0.3	760
Chloromethane	4	4.6	410
Methylene chloride	4	83	2,000
Benzene	3	9.4	270
1,1,1-Trichloroethane	3	5.9	270
1,2-Dichloroethane	3	1.3	1,200

Notes:

    ng/L   =   Nanograms per liter
    PIC   =   Product of incomplete combustion

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TABLE A1.6-3

VOLATILE PICS MOST FREQUENTLY IDENTIFIED IN INCINERATOR EMISSIONS
(OLEXSY, HUFFMAN, AND EVANS 1985)

PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Benzene	6	12	670
Chloroform	5	1	1,330
Tetrachloroethylene	3	0.1	2.5
1,1,1-Trichloroethane	3	0.1	1.5
Toluene	2	2	75
Methylene chloride	2	2	27

Notes:

    ng/L   =   Nanograms per liter
    PIC   =   Product of incomplete combustion

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- From the U.S. EPA-sponsored tests, (1) volatile compounds listed in Appendix VIII identified were only a fraction—sometimes about one-half—of the total organic compounds identified, and (2) semivolatile compounds not listed in Appendix VIII identified were three to 30 times the quantity of organic compounds listed in Appendix VIII . Table A1.6-4 lists the compounds identified by the U.S. EPA-sponsored tests.

- A study of hazardous waste incinerator stack effluent was conducted to characterize the types of compounds emitted. Twenty-nine compounds were identified at a concentration range of 0.1 to 980 nanograms per liter. Methane, chloromethane, and chloroform accounted for more than one-half of the total mass of VOCs detected. Other than methane, oxygenated aliphatic hydrocarbons formed the highest fraction of the total emissions.

- Based on the incinerator stack effluent study, it was found that as combustion conditions deteriorate, increases in mass emissions are first noted with VOCs. Emissions of these compounds, most notably C1 to C3 compounds, increase proportionately more than larger compounds. For larger compounds, available data indicate that emission increases are more likely to be aromatic compounds.

A1.6.3 CARB (1990b)

CARB prepared "Technical Support Document of Proposed Dioxins Control Measures for Medical Waste Incinerators" to meet the requirements of California Health and Safety Code Section 39666 that a needs report be prepared for proposed rules. The report presents a proposed airborne toxic control measure for dioxin emissions from medical waste-burning facilities. The report concentrates on dioxin, furan, and cadmium emissions, although other pollutants detected during the tests are listed. Table A1.6-5 lists these pollutants.

A1.6.4 CARB (1991)

CARB prepared "Air Pollution Control at Resource Recovery Facilities 1991 Update" to update information presented in its 1984 report, entitled "Air Pollution Control at Resource Recovery Facilities." Specifically, the document updates available guidelines concerning incinerator technology, emissions control technology, and emission limits for municipal waste, hospital waste, biomass, tire, manure, landfill and digester gas, and sewer sludge incinerators. The document states that its guidelines represent levels that have been achieved by existing facilities.

In addition, the document summarizes the ultimate analysis of waste types undergoing treatment in the facilities described above. An appendix summarizes stack gas analysis data for numerous operating facilities. Pollutants identified in the analyses are summarized in Table A1.6-6.

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TABLE A1.6-4

MOST FREQUENTLY IDENTIFIED PICS
(TRENHOLM, KAPELLA, AND HINSHAW 1992)

Appendix VIII Volatile Organic Compounds	Appendix VIII Semivolatile Organic Compounds	Compounds Not Listed in Appendix VIII
1,1,1-Trichloroethane	Bis(2-Ethylhexyl)phthalate	1,1'-(1,4-Phenylene)bisethanone
Benzene	Butylbenzylphthalate	Acetone
Carbon tetrachloride	Dibutylphtahlate	Acetophenone
Chlorobenzene	Diethylphthalate	Benzaldehyde
Chloroform	Naphthalene	Benzenedicarboxaldehyde
Methylene chloride	Phenol	Benzoic acid
Tetrachloroethylene		Cyclohexanol
Toluene		Chlorocyclohexanol
Trichloroethylene		Cyclohexane
		Ethylbenzene
		Ethylbenzoic acid
		Ethylphenol
		Ethylphenyl-ethanone
		Ethynylbenzene
		Phenylpropenol
		Propenylmethylbenzene
		Tetramethyloxirane
		Trimethylhexane

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TABLE A1.6-5

COPCS IDENTIFIED BY CARB (1990b)

COPC		
Ammonia	1,2-Dibromoethane	Nickel
Arsenic	Dichloroethane	Nitrogen oxides
Benzene	Dichloromethane	PM
Bromodichloromethane	1,2-Dichloropropane	PAHs
Cadmium	Ethylbenzene	Sulfur dioxide
Carbon dioxide	Freon	Tetrachloroethene
Carbon monoxide	Hydrocarbon, total	Tetratrichloromethylene
Carbon tetrachloride	Hydrogen chloride	Toluene
Chlorobenzenes	Hydrogen fluoride	Tribromomethane
Chlorodibromomethane	Iron	Trichlorethane
Chloroform	Lead	1,1,1-Trichloroethane
Chlorophenols	Manganese	Trichloroethylene
Chromium, hexavalent	Mercury	Trichlorotrifluroethane
Chromium, total	Mesitylene	Vinyl chloride
Copper	Methyl isobutyl ketone	Xylenes
Cumene	Napthalene	Zinc

Notes:

PAH	=	Polynuclear aromatic hydrocarbons
PM	=	Particulate matter

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TABLE A1.6-6

STACK GAS ANALYSIS DATA
(CARB 1991)

(Page 1 of 2)

Pollutant	Incinerator Type [a]						
	Municipal Waste (5)	Hospital Waste (7)	Biomass (4)	Manure (1)	Tire (1)	Landfill Gas (20)	Sewage Sludge and Digester Gas (5)
Nitrogen oxides	✔	✔	✔	✔	✔	✔	✔
Sulfur oxides	✔	✔	ND	✔	✔	✔	✔
Particulate matter	✔	✔	✔	✔	✔	✔	✔
Carbon monoxide	✔	✔	✔	✔	✔	✔	✔
Total hydrocarbons	✔	✔	✔	✔	✔	✔	✔
Hydrogen chloride	✔	✔	NA	NA	✔	NA	NA
Hydrogen fluoride	✔	NA	NA	NA	NA	NA	NA
Amonnia	NA	NA	✔	NA	✔	NA	NA
Carbon dioxide	✔	✔	✔	✔	✔	NA	✔
Oxygen	✔	✔	✔	✔	✔	NA	✔
Arsenic	✔	✔	✔	NA	✔	✔	✔
Beryllium	✔	NA	NA	NA	✔	✔ [b]	✔
Cadmium	✔	✔	✔	NA	ND	✔ [b]	✔
Chromium (total)	✔	✔	✔	NA	✔	✔	✔
Chromium (hexavalent)	ND	✔	NA	NA	✔	NA	NA
Copper	✔	NA	NA	NA	NA	✔	NA
Mercury	✔	✔	NA	NA	ND	✔	✔
Iron	NA	NA	✔	NA	NA	NA	NA
Manganese	NA	NA	✔	NA	NA	NA	NA
Nickel	✔	✔	✔	NA	ND	✔	✔
Lead	✔	✔	✔	NA	ND	✔	✔
Zinc	NA	NA	NA	NA	NA	✔	NA
Polyaromatic hydrocarbons [b]	✔	NA	✔	NA	✔	NA	NA
Polychlorinated biphenyls [b]	✔	ND	✔	NA	✔	NA	NA
CP [b]	✔	NA	✔	NA	✔	NA	NA
CB [b]	✔	NA	✔	NA	✔	NA	NA
Benzene	✔	✔	✔	NA	NA	NA	NA
Polychlorinated dibenzo(p) dioxins [b]	✔	✔	✔	NA	✔	NA	NA
Polychlorinated dibenzofurans [b]	✔	✔	✔	NA	✔	NA	NA
2,3,7,8-Tetrachloro dibenzo(p)dioxin equivalents [b]	✔	✔	✔	NA	✔	NA	✔

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TABLE A1.6-6

STACK GAS ANALYSIS DATA
(CARB 1991)

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Notes:

✔	=	Detected in at least one emission test
ND	=	Not detected in any emission test
NA	=	No analysis

a   Number in parentheses indicates the number of facilities for which data were tabulated.

b   Isomers and/or homologues that were not detected were added to total values at one-half the detection limit; pollutant may not have actually been detected.

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A1.6.5 U.S. EPA (1988)

This document, referenced by some documents as a 1989 document, was prepared in 1988.

U.S. EPA prepared "Hospital Waste Combustion Study: Data Gathering Phase" to assemble available information on hospital waste combustion so that U.S. EPA can evaluate whether airborne pollutant emissions from hospital waste combustion should be regulated. While preparing this document, U.S. EPA reviewed the pertinent literature to determine which studies would be helpful in completing the database on toxic emissions from medical waste incinerators. The report clearly addresses only those pollutants for which emissions data were found. The data reviewed were mostly for larger, controlled air incinerators; and the more commonly used retort incinerators were not evaluated.

The study identified several categories of pollutants that were measured in stack gases; these are discussed in the following paragraphs.

Where evaluated, acid gases were detected in stack gases. For example, HCl was detected in 24 of 28 tests; HCl concentration not recorded in the remaining four tests.

Particulate matter (PM) was detected in all stack tests for 30 facilities at concentrations ranging from 0.001 grains per dry standard cubic foot (gr/dscf), at a facility with PM add-on control devices, to 0.22 gr/dscf at facilities without such control devices.

Trace metals were detected in stack tests for three medical waste incineration facilities. Metals detected include arsenic, cadmium, chromium, iron, manganese, nickel, and lead. The document also states that fine-particle enrichment processes could lead to emissions of molybdenum, tin, selenium, vanadium, and zinc. However, test results for these trace metals are not presented.

With respect to organic emissions, dioxins and furans were detected in emissions from three facilities, both with and without pollution control devices. Other organic emissions detected in stack tests cited in this report include CO, THC, trichlorotrifluoroethane, tetrachloromethane, tetrachloroethene, and trichloroethylene.

In a stack testing conducted on three Canadian biomedical waste incinerators, PCBs and PAHs were either not detected (one facility) or not analyzed (two facilities).

A1.6.6 CARB (1996)

In May 1996, CARB prepared "Proposed Amendments to the Emission Inventory Criteria and Guidelines Report Published in Accordance with the Air Toxics 'Hot Spots' Information and Assessment Act of 1987." The purpose of the report is to present the basis of CARB's recommended amendments to the Air Toxics Hot Spots Program. The report states that California Health and Safety Code (HSC) 44321 requires CARB to compile the list of toxic substances that must be monitored from "designated reference lists of substances." Therefore, the document is not a primary source of toxics emission information. The primary sources of information are mandated by California HSC 44321, as follows:

- California HSC 44321(a): National Toxicology Program, International Agency for Research on Cancer

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- California HSC 44321(b): Governor's List of Carcinogens and Reproductive Toxicants

- California HSC 44321(c): CARB

- California HSC 44321(d): Hazard Evaluation System and Information Service

- California HSC 44321(e): U.S. EPA

- California HSC 44321(f): California HSC

The lists of toxic substances presented in the document are not restricted to incinerator facilities, but apply to any facility discharging airborne pollutants to the atmosphere. The document also removes numerous substances, primarily medicinal compounds, from lists of toxic chemicals that must always be evaluated, and places them on lists of toxic compounds that require evaluation only if a facility manufactures that substance.

A1.7   COLUMN 7: U.S. EPA-RECOMMENDED AND POTENTIAL PICS (1994a; 1994b)

Compounds marked with an "X" in the appropriate cells are identified in U.S. EPA (1994a and 1994b). Based on information presented in U.S. EPA (1994b), these tables were developed from available U.S. EPA data and from lists of toxic compounds from various U.S. EPA programs. Because the source lists were not developed as lists of toxic PICs, U.S. EPA deleted compounds that were not appropriate (U.S. EPA 1994b). U.S. EPA acknowledged the importance of using focused studies to develop a PIC list that is (1) appropriately protective of the environment, and (2) not excessively burdensome on the regulated community. Nevertheless, Tables 1 and 2 in U.S. EPA (1994b) were compiled as draft lists for use during the interim period. Tables in U.S. EPA (1994b) were to be revised as additional PIC data were collected. U.S. EPA Permits and State Program Division is currently updating these tables; however, a target completion date is not available. Tables 1 and 2 are based on the following (U.S. EPA 1994b):

- . Hazardous waste constituent list in 40 CFR Part 261, Appendix VIII

- hazardous air pollutants (HAP) list

- Office of Research and Development list of organic compounds found in combustion devices developed for U.S. EPA (1993)

The following compounds were deleted from this list:

- Pesticide compounds not likely to be a PIC

- Federal Drug Administration-regulated drugs

- Carcinogenic sugar substitutes

- Compounds without chemical-specific listings (for example, "coal tar")

- Compounds without U.S. EPA-established sampling and analysis methods

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- Metallic compounds (because of difficulty in analyzing the specific compounds; metals are still included in elemental totals)

- Compounds with low octanol-water partition coefficients and no inhalation toxicity data

- Compounds with low toxicity values

- Naturally-occurring plant toxins

Specific compounds were retained on Tables 1 and 2 on the following basis:

- Pesticides with a molecular structure simple enough to be of concern as a PIC

- Compounds with very high octanol-water partition coefficients

A1.8   COLUMN 8: PICS ACTUALLY DETECTED IN STACK EMISSIONS

Compounds marked by an "X" in the appropriate cells are PICs that have actually been detected in stack emissions. U.S. EPA compiled this list by evaluating the studies highlighted in Section A1.6.

A1.9   EXAMPLE OF COPC SELECTION PROCESS

As discussed in Chapter 2, seven steps should be followed to identify the COPCs that will be evaluated for each facility. For four of these steps, a sample table—based on data from an existing facility—has been included in this section as an example to illustrate the completion of each step.

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TABLE A1.9-1

STEP 1: IDENTIFY CONCENTRATION DETECTED OR NONDETECT STATUS OF EACH COMPOUND

CAS Number	Compound	Concentration (g/s)
	Total Tetrachlorodibenzofuran	1.34E-10
	Total Pentachlorodibenzofuran	4.71E-11
	Total Hexachlorodibenzofuran	2.25E-11
	Total Heptachlorodibenzofuran	8.33E-11
	2-Methylphenol	<3.16E-7
50-32-8	Benzo(a)pyrene	<5.20E-8
51-28-5	2,4-Dinitrophenol	<1.10E-6
53-70-3	Dibenzo(a,h)anthracene	<5.84E-8
56-23-5	Carbon Tetrachloride	<2.53E-7
56-55-3	Benzo(a)anthracene	<5.40E-8
59-50-7	4-Chloro-3-methlyphenol	<3.74E-7
67-64-1	Acetone	3.79E-7
67-66-3	Chloroform	1.58E-5
67-72-1	Hexachloroethane	<4.06E-7
71-43-2	Benzene	2.97E-5
71-55-6	1,1,1-Trichloroethane	6.10E-7
74-83-9	Bromomethane	<4.19E-7
74-87-3	Chloromethane	<4.11E-7
75-00-3	Chloroethane	<5.76E-7
75-01-4	Vinyl Chloride	<3.67E-7
75-09-2	Methylene Chloride	5.15E-5
75-15-0	Carbon disulfide	<3.67E-7
75-25-2	Bromoform	<3.14E-7

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TABLE A1.9-1

STEP 1: IDENTIFY CONCENTRATION DETECTED OR NONDETECT STATUS OF EACH COMPOUND

CAS Number	Compound	Concentration (g/s)
75-27-4	Bromodichloromethane	<7.03E-7
75-27-4	Dibromochloromethane	<1.83E-7
75-34-3	1,1-Dichloroethane	<1.57E-7
75-69-4	Trichloroflouromethane	4.33E-7
77-47-4	Hexachlorocyclopentadine	<3.11E-7
78-03-3	2-Butanone	<4.50E-6
78-59-1	Isophorone	<1.49E-7
78-87-5	1,2-Dichloropropane	<2.36E-7
79-00-5	Trichloroehtene	2.62E-7
79-00-5	1,1,2-Trichloroethane	<2.61E-7
79-34-5	1,1,2,2-Tetrachloroethane	<2.61E-7
83-32-9	Acenaphthene	<1.34E-7
84-66-1	Diethylphthalate	7.10E-7
84-74-2	Di-n-butylphthalate	1.22E-6
85-01-8	Phenanthrene	<8.32E-8
85-68-7	Butylbenzylphthalate	<8.75E-8
86-30-6	N-Nitrosodiphenylamine	<2.00E-7
86-73-7	Flourene	<1.10E-7
87-68-3	Hexachlorobutadiene	<3.70E-6
87-86-5	Pentochlorophenol	<3.94E-7
88-06-2	2,4,6 -Trichlorophenol	<3.42E-7
88-74-4	2-Nitroaniline	<4.66E-7
88-75-5	2-Nitrophenol	<4.26E-7

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TABLE A1.9-1

STEP 1: IDENTIFY CONCENTRATION DETECTED OR NONDETECT STATUS OF EACH COMPOUND

CAS Number	Compound	Concentration (g/s)
91-20-3	Napthalene	1.18E-6
91-57-6	2-Methylnapthalene	<1.36E-7
91-58-7	2-Chloronapthalene	<1.07E-7
91-94-1	3,3-Dichlorobenzidine	<1.40E-7
95-5-1	1,2-Dichlorobenzene	<2.23E-7
95-47-6	o-xylene	<1.57E-7
95-47-6	Chromium	4.68E-4
95-57-8	2-Chlorophenol	<2.50E-7
95-95-4	2,4,5-Trichlorophenol	<3.29E-7
98-95-3	Nitrobenzene	<2.69E-7
99-09-2	3-Nitroaniline	<4.07E-7
100-01-6	4-Nitroaniline	<3.56E-7
100-02-7	4-Nitrophenol	<6.90-7
100-41-4	Ethylbenzene	<1.83E-7
100-42-5	Styrene	<1.31E-7
100-51-6	Benzyl Alcohol	3.16E-7
101-55-3	4-Bromophenyl-phenylether	<3.99E-7
105-67-9	2,4-Dimethylphenol	<2.97E-7
106-42-3	m-p-Xylene	<1.58E-7
106-45-7	1,4-Dichlorobenzene	<2.05E-7
106-47-8	4-Chloroaniline	<2.08E-7
107-06-2	1,2-Dichloroethane	<1.00E-6
108-05-4	Vinyl Acetate	<1.74E-7

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TABLE A1.9-1

STEP 1: IDENTIFY CONCENTRATION DETECTED OR NONDETECT STATUS OF EACH COMPOUND

CAS Number	Compound	Concentration (g/s)
108-10-1	4-Methyl-2-Pentanone	<4.45E-7
108-39-4	3-Methylphenol	<3.26E-7
108-60-1	2,2 Oxybis (1-Chloropropane)	<3.0E-7
108-88-3	Toluene	2.32E-6
108-90-7	Chlorobenzene	6.97E-7
108-95-2	Phenol	4.39E-7
111-44-4	bis(2-Chloroethyl)ether	<3.19E-7
111-91-1	bis(2-Chloroethoxy)methane	<2.62E-7
117-81-7	bis(2-Ethylhexyl)phthalate	<3.57E-6
117-84-0	Di-n-octylphthalate	<3.51E-8
118-74-1	Hexachlorobenzene	<2.76E-7
120-12-7	anthracene	<9.13E-8
120-82-1	1,2,4-Trichlorobenzene	<4.21E-7
120-83-2	2,4-Dichlorophenol	<3.11E-7
121-14-2	2,4-Dinitrotoluene	<3.28E-7
121-30-6	4,6-Dinitro-2-methyphenol	<5.92E-7
127-18-4	Tetrachloroethene	<2.09E-7
129-00-0	Pyrene	<5.57E-8
131-11-3	Dimethylphthalate	<1.13E-7
132-64-9	Dibenzofuran	<8.09E-7
156-59-2	Cis-1,2-Dichloroethene	<2.36E-7
191-24-2	Benzo(g,h,i)perylene	<4.75E-8
192-97-2	Benzo(e)pyrene	<5.06E-8

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TABLE A1.9-1

STEP 1: IDENTIFY CONCENTRATION DETECTED OR NONDETECT STATUS OF EACH COMPOUND

CAS Number	Compound	Concentration (g/s)
193-39-5	Indeno(1,2,3-cd)pyrene	<4.47E-8
198-55-0	Perylene	<5.57E-8
205-99-2	Benzo(b)fluoranthene	<5.03E-8
206-44-0	Fluoranthene	<6.11E-8
207-08-9	Benzo(k)flouranthene	<5.03E-8
208-96-8	Acenapthylene	<7.52E-8
218-00-0	Chrysene	<5.76E-8
540-59-0	Trans-1,2-Dichloroethene	<2.62E-7
540-59-2	1,2-Dichloroethene	<3.16E-7
541-73-1	1,3-Dichlorobenzene	<2.06E-7
542-75-6	trans-1,3-Dichloropropene	<2.10E-7
542-75-6	cis-1,3-Dichloropropene	<1.57E-7
591-78-6	2-Hexanone	<8.64E-7
606-20-2	2,6-Dinitrotoluene	<4.63E-7
621-64-7	N-Nitroso-di-n-propylamine	<4.62E-7
1090-42-5	Nickel	4.00E-5
1746-01-6	2,3,7,8-Tetrachlorodibenzodioxin	<1.39E-12
3268-87-9	Octachlorodibenzodioxin	1.23E-12
7005-72-3	4-Chlorophenyl-phenylether	<2.26E-7
10408-74-3	1,2,3,7,8,9-Hexachlorodibenzodioxin	<1.39E-12
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzodioxin	5.99E-12
39001-02-0	Total Heptachlorodibenzodioxin	7.82E-12
39227-85-7	1,2,3,4,7,8-Hexachlorodibenzodioxin	<2.70E-12

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TABLE A1.9-1

STEP 1: IDENTIFY CONCENTRATION DETECTED OR NONDETECT STATUS OF EACH COMPOUND

CAS Number	Compound	Concentration (g/s)
55673-89-7	Total Hexachlorodibenzodioxin	2.77E-12
57117-41-6	2,3,4,7,8-Pentachlorodibenzofuran	5.54E-12
57117-41-6	1,2,3,7,8,9-Hexachlorodibenzofuran	<2.77E-12
57117-44-9	1,2,3,4,7,8,9-Heptachlorodibenzofuran	<2.70E-12
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	<1.39E-12
57653-85-7	1,2,3,6,7,8-Hexachlorodibenzodioxin	<1.39E-12
60851-34-5	Octachlorodibenzofuran	8.56E-12
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	8.33E-12
70648-26-9	1,2,3,4,6,7,8-Heptachlorodibenzofuran	1.04E-11
72918-21-9	Total Tetrachlorodibenzodioxin	2.77E-12
7857-2-39-4	Total Pentachlorodibenzodioxin	<1.39E-12
109719-77-9	1,2,3,7,8-Pentachlorodibenzofuran	2.77E-12
109719-77-9	2,3,4,6,7,8-Hexachlorodibenzofuran	5.62E-12
109719-77-9	1,2,3,7,8-Pentachlorodibenzodioxin	<2.70E-12
125322-32-9	2,3,7,8-Tetrachlorodibenxodioxin	1.94E-11

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TABLE A1.9-2A

STEP 2A: IDENTIFY COMPOUNDS PRESENT IN THE WASTE FEED

CAS Number	Compound	Concentration (g/s)
	Total Tetrachlorodibenzofuran	1.34E-10
	Total Pentachlorodibenzofuran	4.71E-11
	Total Hexachlorodibenzofuran	2.25E-11
	Total Heptachlorodibenzofuran	8.33E-11
	2-Methylphenol	<3.16E-7
50-32-8	Benzo(a)pyrene	<5.20E-8
51-28-5	2,4-Dinitrophenol	<1.10E-6
53-70-3	Dibenzo(a,h)anthracene	<5.84E-8
56-23-5	Carbon Tetrachloride	<2.53E-7
56-55-3	Benzo(a)anthracene	<5.40E-8
59-50-7	4-Chloro-3-methlyphenol	<3.74E-7
67-64-1	Acetone	3.79E-7
67-66-3	Chloroform	1.58E-5
67-72-1	Hexachloroethane	<4.06E-7
71-43-2	Benzene	2.97E-5
71-55-6	1,1,1-Trichloroethane	6.10E-7
74-83-9	Bromomethane	<4.19E-7
74-87-3	Chloromethane	<4.11E-7
75-00-3	Chloroethane	<5.76E-7
75-01-4	Vinyl Chloride	<3.67E-7
75-09-2	Methylene Chloride	5.15E-5
75-15-0	Carbon disulfide	<3.67E-7

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TABLE A1.9-2A

STEP 2A: IDENTIFY COMPOUNDS PRESENT IN THE WASTE FEED

CAS Number	Compound	Concentration (g/s)
75-25-2	Bromoform	<3.14E-7
75-27-4	Bromodichloromethane	<7.03E-7
75-27-4	Dibromochloromethane	<1.83E-7
75-34-3	1,1-Dichloroethane	<1.57E-7
75-69-4	Trichloroflouromethane	4.33E-7
77-47-4	Hexachlorocyclopentadine	<3.11E-7
78-03-3	**2-Butanone**	<4.50E-6
78-59-1	Isophorone	<1.49E-7
78-87-5	1,2-Dichloropropane	<2.36E-7
79-00-5	Trichloroehtene	2.62E-7
79-00-5	1,1,2-Trichloroethane	<2.61E-7
79-34-5	1,1,2,2-Tetrachloroethane	<2.61E-7
83-32-9	Acenaphthene	<1.34E-7
84-66-1	Diethylphthalate	7.10E-7
84-74-2	Di-n-butylphthalate	1.22E-6
85-01-8	Phenanthrene	<8.32E-8
85-68-7	Butylbenzylphthalate	<8.75E-8
86-30-6	N-Nitrosodiphenylamine	<2.00E-7
86-73-7	Flourene	<1.10E-7
87-68-3	Hexachlorobutadiene	<3.70E-6
87-86-5	Pentochlorophenol	<3.94E-7
88-06-2	2,4,6 -Trichlorophenol	<3.42E-7

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TABLE A1.9-2A

STEP 2A: IDENTIFY COMPOUNDS PRESENT IN THE WASTE FEED

CAS Number	Compound	Concentration (g/s)
88-74-4	2-Nitroaniline	<4.66E-7
88-75-5	2-Nitrophenol	<4.26E-7
91-20-3	Napthalene	1.18E-6
91-57-6	2-Methylnapthalene	<1.36E-7
91-58-7	2-Chloronapthalene	<1.07E-7
91-94-1	3,3-Dichlorobenzidine	<1.40E-7
95-5-1	1,2-Dichlorobenzene	<2.23E-7
95-47-6	o-xylene	<1.57E-7
95-47-6	**Chromium**	4.68E-4
95-57-8	2-Chlorophenol	<2.50E-7
95-95-4	2,4,5-Trichlorophenol	<3.29E-7
98-95-3	Nitrobenzene	<2.69E-7
99-09-2	3-Nitroaniline	<4.07E-7
100-01-6	4-Nitroaniline	<3.56E-7
100-02-7	4-Nitrophenol	<6.90-7
100-41-4	Ethylbenzene	<1.83E-7
100-42-5	Styrene	<1.31E-7
100-51-6	Benzyl Alcohol	3.16E-7
101-55-3	4-Bromophenyl-phenylether	<3.99E-7
105-67-9	2,4-Dimethylphenol	<2.97E-7
106-42-3	m-p-Xylene	<1.58E-7
106-45-7	1,4-Dichlorobenzene	<2.05E-7

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TABLE A1.9-2A

STEP 2A: IDENTIFY COMPOUNDS PRESENT IN THE WASTE FEED

CAS Number	Compound	Concentration (g/s)
106-47-8	4-Chloroaniline	<2.08E-7
107-06-2	1,2-Dichloroethane	<1.00E-6
108-05-4	Vinyl Acetate	<1.74E-7
108-10-1	4-Methyl-2-Pentanone	<4.45E-7
108-39-4	3-Methylphenol	<3.26E-7
108-60-1	2,2 Oxybis (1-Chloropropane)	<3.0E-7
108-88-3	**Toluene**	2.32E-6
108-90-7	Chlorobenzene	6.97E-7
108-95-2	Phenol	4.39E-7
111-44-4	bis(2-Chloroethyl)ether	<3.19E-7
111-91-1	bis(2-Chloroethoxy)methane	<2.62E-7
117-81-7	bis(2-Ethylhexyl)phthalate	<3.57E-6
117-84-0	Di-n-octylphthalate	<3.51E-8
118-74-1	Hexachlorobenzene	<2.76E-7
120-12-7	anthracene	<9.13E-8
120-82-1	1,2,4-Trichlorobenzene	<4.21E-7
120-83-2	2,4-Dichlorophenol	<3.11E-7
121-14-2	2,4-Dinitrotoluene	<3.28E-7
121-30-6	4,6-Dinitro-2-methyphenol	<5.92E-7
127-18-4	Tetrachloroethene	<2.09E-7
129-00-0	Pyrene	<5.57E-8
131-11-3	Dimethylphthalate	<1.13E-7

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TABLE A1.9-2A

STEP 2A: IDENTIFY COMPOUNDS PRESENT IN THE WASTE FEED

CAS Number	Compound	Concentration (g/s)
132-64-9	Dibenzofuran	<8.09E-7
156-59-2	Cis-1,2-Dichloroethene	<2.36E-7
191-24-2	Benzo(g,h,i)perylene	<4.75E-8
192-97-2	Benzo(e)pyrene	<5.06E-8
193-39-5	Indeno(1,2,3-cd)pyrene	<4.47E-8
198-55-0	Perylene	<5.57E-8
205-99-2	Benzo(b)fluoranthene	<5.03E-8
206-44-0	Fluoranthene	<6.11E-8
207-08-9	Benzo(k)flouranthene	<5.03E-8
208-96-8	Acenapthylene	<7.52E-8
218-00-0	Chrysene	<5.76E-8
540-59-0	Trans-1,2-Dichloroethene	<2.62E-7
540-59-2	1,2-Dichloroethene	<3.16E-7
541-73-1	1,3-Dichlorobenzene	<2.06E-7
542-75-6	trans-1,3-Dichloropropene	<2.10E-7
542-75-6	cis-1,3-Dichloropropene	<1.57E-7
591-78-6	2-Hexanone	<8.64E-7
606-20-2	2,6-Dinitrotoluene	<4.63E-7
621-64-7	N-Nitroso-di-n-propylamine	<4.62E-7
1090-42-5	**Nickel**	4.00E-5
1746-01-6	2,3,7,8-Tetrachlorodibenzodioxin	<1.39E-12
3268-87-9	Octachlorodibenzodioxin	1.23E-12

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TABLE A1.9-2A

STEP 2A: IDENTIFY COMPOUNDS PRESENT IN THE WASTE FEED

CAS Number	Compound	Concentration (g/s)
7005-72-3	4-Chlorophenyl-phenylether	<2.26E-7
10408-74-3	1,2,3,7,8,9-Hexachlorodibenzodioxin	<1.39E-12
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzodioxin	5.99E-12
39001-02-0	Total Heptachlorodibenzodioxin	7.82E-12
39227-85-7	1,2,3,4,7,8-Hexachlorodibenzodioxin	<2.70E-12
55673-89-7	Total Hexachlorodibenzodioxin	2.77E-12
57117-41-6	2,3,4,7,8-Pentachlorodibenzofuran	5.54E-12
57117-41-6	1,2,3,7,8,9-Hexachlorodibenzofuran	<2.77E-12
57117-44-9	1,2,3,4,7,8,9-Heptachlorodibenzofuran	<2.70E-12
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	<1.39E-12
57653-85-7	1,2,3,6,7,8-Hexachlorodibenzodioxin	<1.39E-12
60851-34-5	Octachlorodibenzofuran	8.56E-12
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	8.33E-12
70648-26-9	1,2,3,4,6,7,8-Heptachlorodibenzofuran	1.04E-11
72918-21-9	Total Tetrachlorodibenzodioxin	2.77E-12
7857-2-39-4	Total Pentachlorodibenzodioxin	<1.39E-12
109719-77-9	1,2,3,7,8-Pentachlorodibenzofuran	2.77E-12
109719-77-9	2,3,4,6,7,8-Hexachlorodibenzofuran	5.62E-12
109719-77-9	1,2,3,7,8-Pentachlorodibenzodioxin	<2.70E-12
125322-32-9	2,3,7,8-Tetrachlorodibenxodioxin	1.94E-11

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TABLE A-1.9-2B

STEP 2B: LIST COMPONENTS IN WASTE FEED

CAS Number	Compound	CAS Number	Compound
64-17-5	Ethanol	7440-02-0	Nickel
65-53-3	Aniline	7440-47-3	Chromium
67-5-1	Methanol	208030-75-5	Dioctylamine
67-63-0	Isopropyl alcohol	- - -	Bisaminopropylmethylamine
71-36-8	Butanol	- - -	1,3-Diaminopropane
74-89-5	Methylamine		Diethylbutylamine
75-04-7	Ethylamine	- - -	1,2-Diaminopropane
78-83-3	Methyl ethyl ketone (2-Butanone)	- - -	Dimethylamino propylamine
78-96-6	Isopropanol amine	- - -	3-Dimethylamino propylamine
107-10-8	Propylamine	- - -	Dimethylcyclohexylamine
108-94-1	Cyclohexanone	- - -	Ethoxypropylamine
109-02-4	Methylmorpholine	- - -	Ethyl dimethyl propylamine
109-89-7	Diethylamine	- - -	Methaminepropamine
109-99-9	Tetrahydrofuran	- - -	Methyl cyclohexylamine
110-89-4	Piperdine	- - -	Methocypropylamine
110-91-8	Morpholine	- - -	3-Methoxypropinitrite
111-29-5	Pentanediol	- - -	Methyl piperdine
111-46-6	Diethylene glycol	- - -	Imino-bis-propylamine
111-87-5	Octanol	- - -	Octylamine
137-32-6	Methylbutanol	- - -	Trioctylamine
814-78-8	Methyl isopropyl ketone	- - -	mono-Trioxatridecanediamine
1484-89-6	Ethyl piperdine	- - -	Trioxatridecanediamine

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TABLE A-1.9-3

STEP 3: DELETE NONDETECTED COMPOUNDS WITH NO TOXICOLOGICAL DATA

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
	Total Tetrachlorodibenzofuran	1.34E-10	
	Total Pentachlorodibenzofuran	4.71E-11	
	Total Hexachlorodibenzofuran	2.25E-11	
	Total Heptachlorodibenzofuran	8.33E-11	
	2-Methylphenol	<3.16E-7	
50-32-8	Benzo(a)pyrene	<5.20E-8	
51-28-5	2,4-Dinitrophenol	<1.10E-6	
53-70-3	Dibenzo(a,h)anthracene	<5.84E-8	
56-23-5	Carbon Tetrachloride	<2.53E-7	
56-55-3	Benzo(a)anthracene	<5.40E-8	
59-50-7	4-Chloro-3-methlyphenol	<3.74E-7	No toxicological data
67-64-1	Acetone	3.79E-7	
67-66-3	Chloroform	1.58E-5	
67-72-1	Hexachloroethane	<4.06E-7	
71-43-2	Benzene	2.97E-5	
71-55-6	1,1,1-Trichloroethane	6.10E-7	
74-83-9	Bromomethane	<4.19E-7	
74-87-3	Chloromethane	<4.11E-7	
75-00-3	Chloroethane	<5.76E-7	No toxicological data
75-01-4	Vinyl Chloride	<3.67E-7	
75-09-2	Methylene Chloride	5.15E-5	
75-15-0	Carbon disulfide	<3.67E-7	

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TABLE A-1.9-3

STEP 3: DELETE NONDETECTED COMPOUNDS WITH NO TOXICOLOGICAL DATA

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
75-25-2	Bromoform	<3.14E-7	
75-27-4	Bromodichloromethane	<7.03E-7	
75-27-4	Dibromochloromethane	<1.83E-7	
75-34-3	1,1-Dichloroethane	<1.57E-7	
75-69-4	Trichloroflouromethane	4.33E-7	
77-47-4	Hexachlorocyclopentadine	<3.11E-7	
78-03-3	2-Butanone	<4.50E-6	
78-59-1	Isophorone	<1.49E-7	No toxicological data
78-87-5	1,2-Dichloropropane	<2.36E-7	
79-00-5	Trichloroehtene	2.62E-7	
79-00-5	1,1,2-Trichloroethane	<2.61E-7	
79-34-5	1,1,2,2-Tetrachloroethane	<2.61E-7	
83-32-9	Acenaphthene	<1.34E-7	No toxicological data
84-66-1	Diethylphthalate	7.10E-7	
84-74-2	Di-n-butylphthalate	1.22E-6	
85-01-8	Phenanthrene	<8.32E-8	
85-68-7	Butylbenzylphthalate	<8.75E-8	
86-30-6	N-Nitrosodiphenylamine	<2.00E-7	No toxicological data
86-73-7	Flourene	<1.10E-7	No toxicological data
87-68-3	Hexachlorobutadiene	<3.70E-6	
87-86-5	Pentochlorophenol	<3.94E-7	

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TABLE A-1.9-3

STEP 3: DELETE NONDETECTED COMPOUNDS WITH NO TOXICOLOGICAL DATA

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
88-06-2	2,4,6 -Trichlorophenol	<3.42E-7	
88-74-4	2-Nitroaniline	<4.66E-7	No toxicological data
88-75-5	2-Nitrophenol	<4.26E-7	No toxicological data
91-20-3	Napthalene	1.18E-6	
91-57-6	2-Methylnapthalene	<1.36E-7	No toxicological data
91-58-7	2-Chloronapthalene	<1.07E-7	
91-94-1	3,3-Dichlorobenzidine	<1.40E-7	
95-5-1	1,2-Dichlorobenzene	<2.23E-7	
95-47-6	o-xylene	<1.57E-7	
95-47-6	Chromium[1]	4.68E-4	
95-57-8	2-Chlorophenol	<2.50E-7	
95-95-4	2,4,5-Trichlorophenol	<3.29E-7	
98-95-3	Nitrobenzene	<2.69E-7	
99-09-2	3-Nitroaniline	<4.07E-7	No toxicological data
100-01-6	4-Nitroaniline	<3.56E-7	No toxicological data
100-02-7	4-Nitrophenol	<6.90-7	No toxicological data
100-41-4	Ethylbenzene	<1.83E-7	
100-42-5	Styrene	<1.31E-7	

[1]Emission rate based on waste feed rate.

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TABLE A-1.9-3

STEP 3: DELETE NONDETECTED COMPOUNDS WITH NO TOXICOLOGICAL DATA

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
100-51-6	Benzyl Alcohol	3.16E-7	
101-55-3	4-Bromophenyl-phenylether	<3.99E-7	No toxicological data
105-67-9	2,4-Dimethylphenol	<2.97E-7	No toxicological data
106-42-3	m-p-Xylene	<1.58E-7	
106-45-7	1,4-Dichlorobenzene	<2.05E-7	
106-47-8	4-Chloroaniline	<2.08E-7	
107-06-2	1,2-Dichloroethane	<1.00E-6	
108-05-4	Vinyl Acetate	<1.74E-7	
108-10-1	4-Methyl-2-Pentanone	<4.45E-7	
108-39-4	3-Methylphenol	<3.26E-7	
108-60-1	2,2-Oxybis (1-Chloropropane)	<3.0E-7	No toxicological data
108-88-3	**Toluene**	2.32E-6	
108-90-7	Chlorobenzene	6.97E-7	
108-95-2	Phenol	4.39E-7	
111-44-4	bis(2-Chloroethyl)ether	<3.19E-7	
111-91-1	bis(2-Chloroethoxy)methane	<2.62E-7	No toxicological data
117-81-7	bis(2-Ethylhexyl)phthalate	<3.57E-6	
117-84-0	Di-n-octylphthalate	<3.51E-8	
118-74-1	Hexachlorobenzene	<2.76E-7	No toxicological data
120-12-7	Anthracene	<9.13E-8	

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TABLE A-1.9-3

STEP 3: DELETE NONDETECTED COMPOUNDS WITH NO TOXICOLOGICAL DATA

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
120-82-1	1,2,4-Trichlorobenzene	<4.21E-7	
120-83-2	2,4-Dichlorophenol	<3.11E-7	
121-14-2	2,4-Dinitrotoluene	<3.28E-7	
121-30-6	4,6-Dinitro-2-methyphenol	<5.92E-7	
127-18-4	Tetrachloroethene	<2.09E-7	
129-00-0	Pyrene	<5.57E-8	
131-11-3	Dimethylphthalate	<1.13E-7	
132-64-9	~~Dibenzofuran~~	<8.09E-7	No toxicological data
156-59-2	Cis-1,2-Dichloroethene	<2.36E-7	
191-24-2	Benzo(g,h,i)perylene	<4.75E-8	
192-97-2	Benzo(e)pyrene	<5.06E-8	
193-39-5	Indeno(1,2,3-cd)pyrene	<4.47E-8	
198-55-0	Perylene	<5.57E-8	
205-99-2	Benzo(b)fluoranthene	<5.03E-8	
206-44-0	Fluoranthene	<6.11E-8	
207-08-9	Benzo(k)flouranthene	<5.03E-8	
208-96-8	~~Acenapthylene~~	<7.52E-8	No toxicological data
218-00-0	Chrysene	<5.76E-8	
540-59-0	Trans-1,2-Dichloroethene	<2.62E-7	
540-59-2	1,2-Dichloroethene	<3.16E-7	
541-73-1	1,3-Dichlorobenzene	<2.06E-7	
542-75-6	trans-1,3-Dichloropropene	<2.10E-7	

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TABLE A-1.9-3

STEP 3: DELETE NONDETECTED COMPOUNDS WITH NO TOXICOLOGICAL DATA

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
542-75-6	cis-1,3-Dichloropropene	<1.57E-7	
591-78-6	2-Hexanone	<8.64E-7	No toxicological data
606-20-2	2,6-Dinitrotoluene	<4.63E-7	
621-64-7	N-Nitroso-di-n-propylamine	<4.62E-7	
1090-42-5	Nickel[1]	4.00E-5	
1746-01-6	2,3,7,8-Tetrachlorodibenzodioxin	<1.39E-12	
3268-87-9	Octachlorodibenzodioxin	1.23E-12	
7005-72-3	4-Chlorophenyl-phenylether	<2.26E-7	No toxicological data
10408-74-3	1,2,3,7,8,9-Hexachlorodibenzodioxin	<1.39E-12	
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzodioxin	5.99E-12	
39001-02-0	Total Heptachlorodibenzodioxin	7.82E-12	
39227-85-7	1,2,3,4,7,8-Hexachlorodibenzodioxin	<2.70E-12	
55673-89-7	Total Hexachlorodibenzodioxin	2.77E-12	
57117-41-6	2,3,4,7,8-Pentachlorodibenzofuran	5.54E-12	
57117-41-6	1,2,3,7,8,9-Hexachlorodibenzofuran	<2.77E-12	
57117-44-9	1,2,3,4,7,8,9-Heptachlorodibenzofuran	<2.70E-12	
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	<1.39E-12	
57653-85-7	1,2,3,6,7,8-Hexachlorodibenzodioxin	<1.39E-12	
60851-34-5	Octachlorodibenzofuran	8.56E-12	
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	8.33E-12	
70648-26-9	1,2,3,4,6,7,8-Heptachlorodibenzofuran	1.04E-11	
72918-21-9	Total Tetrachlorodibenzodioxin	2.77E-12	

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TABLE A-1.9-3

STEP 3: DELETE NONDETECTED COMPOUNDS WITH NO TOXICOLOGICAL DATA

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
7857-2-39-4	Total Pentachlorodibenzodioxin	<1.39E-12	
109719-77-9	1,2,3,7,8-Pentachlorodibenzofuran	2.77E-12	
109719-77-9	2,3,4,6,7,8-Hexachlorodibenzofuran	5.62E-12	
109719-77-9	1,2,3,7,8-Pentachlorodibenzodioxin	<2.70E-12	
125322-32-9	2,3,7,8-Tetrachlorodibenxodioxin	1.94E-11	

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TABLE A-1.9-4

STEP 4: DELETE COMPOUNDS NOT EXPECTED IN STACK EMISSIONS

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
	Total Tetrachlorodibenzofuran	1.34E-10	
	Total Pentachlorodibenzofuran	4.71E-11	
	Total Hexachlorodibenzofuran	2.25E-11	
	Total Heptachlorodibenzofuran	8.33E-11	
	2-Methylphenol	<3.16E-7	
50-32-8	Benzo(a)pyrene	<5.20E-8	
51-28-5	2,4-Dinitrophenol	<1.10E-6	
53-70-3	Dibenzo(a,h)anthracene	<5.84E-8	
56-23-5	Carbon Tetrachloride	<2.53E-7	Chlorinated compounds not used at facility.
56-55-3	Benzo(a)anthracene	<5.40E-8	
59-50-7	4-Chloro-3-methlyphenol	<3.74E-7	No toxicological data
67-64-1	Acetone	3.79E-7	
67-66-3	Chloroform	1.58E-5	
67-72-1	Hexachloroethane	<4.06E-7	Chlorinated compounds not used at facility.
71-43-2	Benzene	2.97E-5	
71-55-6	1,1,1-Trichloroethane	6.10E-7	
74-83-9	Bromomethane	<4.19E-7	
74-87-3	Chloromethane	<4.11E-7	Chlorinated compounds not used at facility.
75-00-3	Chloroethane	<5.76E-7	No toxicological data

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TABLE A-1.9-4

STEP 4: DELETE COMPOUNDS NOT EXPECTED IN STACK EMISSIONS

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
75-01-4	~~Vinyl Chloride~~	<3.67E-7	Chlorinated compounds not used at facility.
75-09-2	Methylene Chloride	5.15E-5	
75-15-0	Carbon disulfide	<3.67E-7	
75-25-2	Bromoform	<3.14E-7	
75-27-4	~~Dibromochloromethane~~	<1.83E-7	Chlorinated compounds not used at facility.
75-27-4	~~Bromodichloromethane~~	<7.03E-7	Chlorinated compounds not used at facility.
75-34-3	1,1-Dichloroethane	<1.57E-7	
75-69-4	Trichloroflouromethane	4.33E-7	
77-47-4	~~Hexachlorocyclopentadine~~	<3.11E-7	Chlorinated compounds not used at facility.
78-03-3	2-Butanone	<4.50E-6	
78-59-1	~~Isophorone~~	<1.49E-7	No toxicological data
78-87-5	~~1,2-Dichloropropane~~	<2.36E-7	Chlorinated compounds not used at facility.
79-00-5	Trichloroehtene	2.62E-7	
79-00-5	~~1,1,2-Trichloroethane~~	<2.61E-7	Chlorinated compounds not used at facility.

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TABLE A-1.9-4

STEP 4: DELETE COMPOUNDS NOT EXPECTED IN STACK EMISSIONS

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
79-34-5	1,1,2,2-Tetrachloroethane	<2.61E-7	Chlorinated compounds not used at facility.
83-32-9	Acenaphthene	<1.34E-7	No toxicological data
84-66-1	Diethylphthalate	7.10E-7	
84-74-2	Di-n-butylphthalate	1.22E-6	
85-01-8	Phenanthrene	<8.32E-8	
85-68-7	Butylbenzylphthalate	<8.75E-8	
86-30-6	N-Nitrosodiphenylamine	<2.00E-7	No toxicological data
86-73-7	Flourene	<1.10E-7	No toxicological data
87-68-3	Hexachlorobutadiene	<3.70E-6	Chlorinated compounds not used at facility.
87-86-5	Pentochlorophenol	<3.94E-7	Chlorinated compounds not used at facility.
88-06-2	2,4,6-Trichlorophenol	<3.42E-7	Chlorinated compounds not used at facility.
88-74-4	2-Nitroaniline	<4.66E-7	No toxicological data
88-75-5	2-Nitrophenol	<4.26E-7	No toxicological data
91-20-3	Napthalene	1.18E-6	
91-57-6	2-Methylnapthalene	<1.36E-7	No toxicological data

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TABLE A-1.9-4

STEP 4: DELETE COMPOUNDS NOT EXPECTED IN STACK EMISSIONS

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
91-58-7	2-Chloronapthalene	<1.07E-7	Chlorinated compounds not used at facility.
91-94-1	3,3-Dichlorobenzidine	<1.40E-7	Chlorinated compounds not used at facility.
95-5-1	1,2-Dichlorobenzene	<2.23E-7	Chlorinated compounds not used at facility.
95-47-6	**Chromium**	4.68E-4	
95-47-6	o-xylene	<1.57E-7	
95-57-8	2-Chlorophenol	<2.50E-7	Chlorinated compounds not used at facility.
95-95-4	2,4,5-Trichlorophenol	<3.29E-7	Chlorinated compounds not used at facility.
98-95-3	Nitrobenzene	<2.69E-7	
99-09-2	3-Nitroaniline	<4.07E-7	No toxicological data
100-01-6	4-Nitroaniline	<3.56E-7	No toxicological data
100-02-7	4-Nitrophenol	<6.90-7	No toxicological data
100-41-4	Ethylbenzene	<1.83E-7	
100-42-5	Styrene	<1.31E-7	
100-51-6	Benzyl Alcohol	3.16E-7	
101-55-3	4-Bromophenyl-phenylether	<3.99E-7	No toxicological data

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TABLE A-1.9-4

STEP 4: DELETE COMPOUNDS NOT EXPECTED IN STACK EMISSIONS

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
105-67-9	2,4-Dimethylphenol	<2.97E-7	No toxicological data
106-42-3	m-p-Xylene	<1.58E-7	
106-45-7	1,4-Dichlorobenzene	<2.05E-7	Chlorinated compounds not used at facility.
106-47-8	4-Chloroaniline	<2.08E-7	Chlorinated compounds not used at facility.
107-06-2	1,2-Dichloroethane	<1.00E-6	
108-05-4	Vinyl Acetate	<1.74E-7	
108-10-1	4-Methyl-2-Pentanone	<4.45E-7	
108-39-4	3-Methylphenol	<3.26E-7	
108-60-1	2,2-Oxybis (1-Chloropropane)	<3.0E-7	No toxicological data
108-88-3	**Toluene**	2.32E-6	
108-90-7	Chlorobenzene	6.97E-7	
108-95-2	Phenol	4.39E-7	
111-44-4	bis(2-Chloroethyl)ether	<3.19E-7	Chlorinated compounds not used at facility.
111-91-1	bis(2-Chloroethoxy)methane	<2.62E-7	No toxicological data
117-81-7	bis(2-Ethylhexyl)phthalate	<3.57E-6	
117-84-0	Di-n-octylphthalate	<3.51E-8	
118-74-1	Hexachlorobenzene	<2.76E-7	No toxicological data

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TABLE A-1.9-4

STEP 4: DELETE COMPOUNDS NOT EXPECTED IN STACK EMISSIONS

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
120-12-7	Anthracene	<9.13E-8	
120-82-1	1,2,4-Trichlorobenzene	<4.21E-7	Chlorinated compounds not used at facility.
120-83-2	2,4-Dichlorophenol	<3.11E-7	Chlorinated compounds not used at facility.
121-14-2	2,4-Dinitrotoluene	<3.28E-7	
121-30-6	4,6-Dinitro-2-methyphenol	<5.92E-7	
127-18-4	Tetrachloroethene	<2.09E-7	
129-00-0	Pyrene	<5.57E-8	
131-11-3	Dimethylphthalate	<1.13E-7	
132-64-9	Dibenzofuran	<8.09E-7	No toxicological data
156-59-2	Cis-1,2-Dichloroethene	<2.36E-7	
191-24-2	Benzo(g,h,i)perylene	<4.75E-8	
192-97-2	Benzo(e)pyrene	<5.06E-8	
193-39-5	Indeno(1,2,3-cd)pyrene	<4.47E-8	
198-55-0	Perylene	<5.57E-8	
205-99-2	Benzo(b)fluoranthene	<5.03E-8	
206-44-0	Fluoranthene	<6.11E-8	
207-08-9	Benzo(k)flouranthene	<5.03E-8	
208-96-8	Acenapthylene	<7.52E-8	No toxicological data
218-00-0	Chrysene	<5.76E-8	
540-59-0	Trans-1,2-Dichloroethene	<2.62E-7	

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TABLE A-1.9-4

STEP 4: DELETE COMPOUNDS NOT EXPECTED IN STACK EMISSIONS

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
540-59-2	1,2-Dichloroethene	<3.16E-7	
541-73-1	1,3-Dichlorobenzene	<2.06E-7	Chlorinated compounds not used at facility.
542-75-6	trans-1,3-Dichloropropene	<2.10E-7	Chlorinated compounds not used at facility.
542-75-6	cis-1,3-Dichloropropene	<1.57E-7	Chlorinated compounds not used at facility.
591-78-6	2-Hexanone	<8.64E-7	No toxicological data
606-20-2	2,6-Dinitrotoluene	<4.63E-7	
621-64-7	N-Nitroso-di-n-propylamine	<4.62E-7	
1090-42-5	Nickel	4.00E-5	
1746-01-6	2,3,7,8-Tetrachlorodibenzodioxin	<1.39E-12	
3268-87-9	Octachlorodibenzodioxin	1.23E-12	
7005-72-3	4-Chlorophenyl-phenylether	<2.26E-7	No toxicological data
10408-74-3	1,2,3,7,8,9-Hexachlorodibenzodioxin	<1.39E-12	
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzodioxin	5.99E-12	
39001-02-0	Total Heptachlorodibenzodioxin	7.82E-12	
39227-85-7	1,2,3,4,7,8-Hexachlorodibenzodioxin	<2.70E-12	
55673-89-7	Total Hexachlorodibenzodioxin	2.77E-12	
57117-41-6	2,3,4,7,8-Pentachlorodibenzofuran	5.54E-12	
57117-41-6	1,2,3,7,8,9-Hexachlorodibenzofuran	<2.77E-12	
57117-44-9	1,2,3,4,7,8,9-Heptachlorodibenzofuran	<2.70E-12	

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TABLE A-1.9-4

STEP 4: DELETE COMPOUNDS NOT EXPECTED IN STACK EMISSIONS

CAS Number	Compound	Concentration (g/s)	Rationale for Deletion
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	<1.39E-12	
57653-85-7	1,2,3,6,7,8-Hexachlorodibenzodioxin	<1.39E-12	
60851-34-5	Octachlorodibenzofuran	8.56E-12	
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	8.33E-12	
70648-26-9	1,2,3,4,6,7,8-Heptachlorodibenzofuran	1.04E-11	
72918-21-9	Total Tetrachlorodibenzodioxin	2.77E-12	
7857-2-39-4	Total Pentachlorodibenzodioxin	<1.39E-12	
109719-77-9	1,2,3,7,8-Pentachlorodibenzofuran	2.77E-12	
109719-77-9	2,3,4,6,7,8-Hexachlorodibenzofuran	5.62E-12	
109719-77-9	1,2,3,7,8-Pentachlorodibenzodioxin	<2.70E-12	
125322-32-9	2,3,7,8-Tetrachlorodibenxodioxin	1.94E-11	

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California Air Resources Board (CARB). 1990a. "Health Risk Assessment Guidelines for Nonhazardous Waste Incinerators." Prepared by the Stationary Source Division of the CARB and the California Department of Health Services.

CARB. 1990b. "Technical Support Document of Proposed Dioxins Control Measures for Medical Waste Incinerators." May 25.

CARB. 1991. "Air Pollution Control at Resource Recovery Facilities. Update."

CARB. 1996. "Proposed Amendments to the Emission Inventory Criteria and Guidelines Report Published in Accordance with the Air Toxics 'Hot Spots' Information and Assessment Act of 1987." May.

Castaldini, C., and others. 1984. "Engineering Assessment Report—Hazardous Waste Cofiring in Industrial Boilers." Report to U.S. Environmental Protection Agency under Contract No. 68-02-3188. June.

Dellinger, B., D.L. Hall, J.L. Graham, S.L. Mazer, W.A. Rubey, and M. Malanchuk. 1986. *PIC Formation Under Pyrolytic and Starved Air Conditions.*. Prepared for the U.S. EPA Industrial Environmental Research Laboratory. Prepared by the University of Dayton Research Institute. EPA/600/2-86/006. NTIS PB-86-145422. January.

Dellinger, B., J.L. Torres, W.A. Rubey, D.L. Hall, and J.L. Graham. 1984. *Determination of the Thermal Decomposition Properties of 20 Selected Hazardous Organic Compounds.* Prepared for the U.S. EPA Industrial Environmental Research Laboratory. Prepared by the University of Dayton Research Institute. EPA-600/2-84-138. NTIS PB-84-232487. August.

Demsey, C.R., and E.T. Oppelt. 1993. "Incineration of Hazardous Waste: A Critical Review Update." *Air and Waste.* 43:25-73.

Duval, D.S., and W.A. Rubey. 1976. *Laboratory Evaluation of High-Temperature Destruction of Kepone and Related Pesticides.* EPA-600/2-76-299. NTIS PB-264892/1. December.

Duval, D.S., and W.A. Rubey. 1977. *Laboratory Evaluation of High-Temperature Destruction of Polychlorinated Biphenyls and Related Compounds.* EPA-600/2-77-228. NTIS PB-279139/0. December.

Kramlich, J.C., W.R. Seeker, and M.P. Heap. 1984. "Laboratory-Scale Flame Mode Study of Hazardous Waste Incineration." *Proceedings of the Ninth Annual Research Symposium on Incineration and Treatment of Hazardous Waste.* Fort Mitchell, Kentucky. May 2 through 4, 1983. EPA-600/9-84/015. NTIS PB-84-234525. Pages 79-94. July.

U.S. EPA Region 6
Multimedia Planning and Permitting Division
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U.S. EPA
Office of Solid Waste
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Olexsey, R.A., G.L. Huffman, and G.M. Evans. 1985. "Emission and Control of By-Products from Hazardous Waste Combustion Processes." *Proceedings of the 11th Annual Research Symposium on Incineration and Treatment of Hazardous Waste*. Cincinnati, Ohio. April 29 to May 1, 1985. EPA-600/9-85/028. NTIS PB-86-199403. Pages 8-15. September.

Trenholm, A., and R. Hathaway. 1984. "Products of Incomplete Combustion from Hazardous Waste Incinerators." *Proceedings of the 10th Annual Research Symposium on Incineration and Treatment of Hazardous Waste. Fort Mitchell, Kentucky. April 3-5.* EPA-600/9-84/022. NTIS PB-85-116291. Pages 84-95. September.

Trenholm, Andrew R., David W. Kapella, and Gary D. Hinshaw. 1992. "Organic Products of Incomplete Combustion from Hazardous Waste Combustion." *Proceedings of the Air and Waste Management Association 85th Annual Meeting and Exhibition*. Kansas City, Missouri. June 21-26.

Trenholm, A., and C.C. Lee. 1986. "Analysis of PIC and Total Mass Emissions from an Incinerator." *Proceedings of the Twelfth Annual Research Symposium on Land Disposal, Remedial Action, Incineration, and Treatment of Hazardous Waste*. Cincinnati, Ohio. April 21 to 23, 1986. EPA/60-9-86/022. Pages 376-381. August.

Trenholm, A., and others. 1984. "Performance Evaluation of Full-Scale Hazardous Waste Incinerators." Report to U.S. EPA under Contract No. 68-02-3177.

U.S. Environmental Protection Agency (EPA). 1981. "Incinerator Standards for Owners and Operators of Hazardous Waste Management Facilities; Interim Final Rule and Proposed Rule." *Federal Register*. 46(15):7666-7690. January 23.

U.S. EPA. 1985. *Report on the Incineration of Liquid Hazardous Wastes*. Science Advisory Board. Environmental Effects, Transport, and Fate Committee. April.

U.S. EPA. 1987. *Total Mass Emissions from a Hazardous Waste Incinerator*. Final Report. Midwest Research Institute. EPA-600/S2-87/064. NTIS PB-87-228508/AS. June 12.

U.S. EPA. 1988. "Hospital Waste Combustion Study: Data Gathering Phase." Office of Air Quality Planning and Standards. Research Triangle Park, North Carolina. EPA-450/3-88-008. December.

U.S. EPA. 1989. *Guidance of PIC Controls for Hazardous Waste Incinerators. Volume V of the Hazardous Waste Incineration Guidance Series*. EPA/530-SW-90-040. April 3.

U.S. EPA. 1990a. "Standards for Owners and Operators of Hazardous Waste Incinerators and Burning of Hazardous Wastes in Boilers and Industrial Furnaces; Proposed Rule, Supplemental Proposed Rule, Technical Corrections, and Request for Comments." *Federal Register*. 55(82):17862-17921. April 27.

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U.S. EPA. 1990b. *Report of the Products of Incomplete Combustion Subcommittee of the Science Advisory Board; Review of OSW Proposed Controls for Hazardous Waste Incineration Products of Incomplete Combustion.* EPA-SAB EC-90-004. October 24.

U.S. EPA. 1993. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* OHEA. ORD. EPA-600-AP-93-003. November 10.

U.S. EPA. 1994a. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes: Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* Office of Emergency and Remedial Response (OERR). OSW. December 14.

U.S. EPA. 1994b. "Table 1—Chemicals Recommended for Identification and Table 2—Chemicals for Potential Identification." *Draft Exposure Assessment Guidance for Resource Conservation and Recovery Act Hazardous Waste Combustion Facilities: Attachment.* April 15.

U.S. EPA. 1995. "Basis for Listing Hazardous Waste.: *Title 40, Code of Federal Regulations, Part 261, Appendices VII and VIII.*

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APPENDIX A-2

TARGET ORGANS AND CRITICAL EFFECTS
FOR COMPOUNDS WITH REFERENCE DOSE VALUES
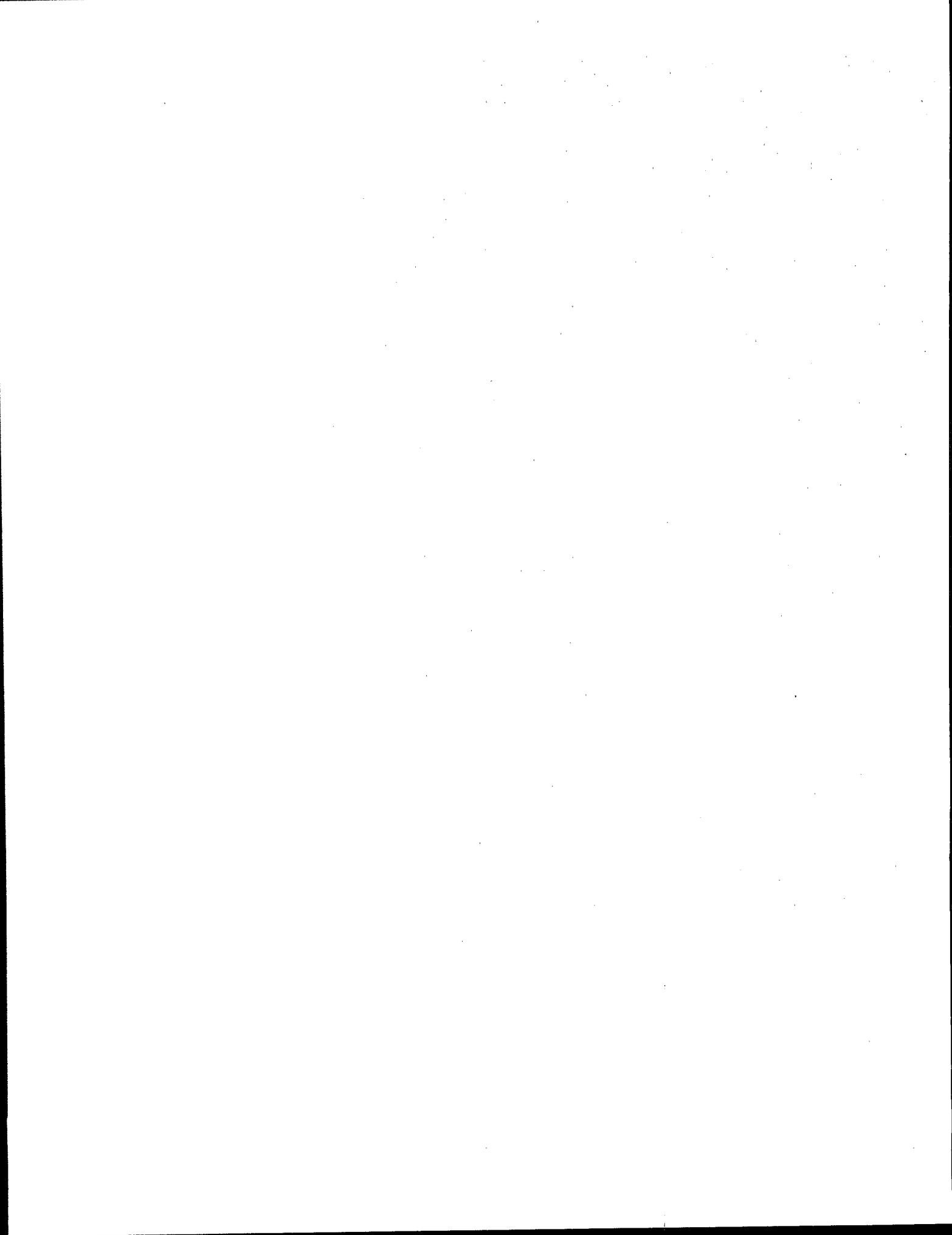
TABLE A-2

TARGET ORGANS AND CRITICAL EFFECTS
FOR COMPOUNDS WITH REFERENCE DOSE VALUES

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Compound	CAS No.	Target Organ	Critical Effect
Acenaphthene	83-32-9	Liver	Hepatotoxicity
Acetone	67-64-1	Liver	Increased liver weights
		Kidney	Increased kidney weights and nephrotoxicity
Acetonitrile	75-05-8	Blood	Decreased red blood cell counts and hematocrit
		Liver	Hepatic lesions
Acetophenone	98-86-2	General	General toxicity
Acrolein	107-02-8	--	No adverse effects observed
Acrylonitrile	107-13-1	Reproductive	Decreased sperm counts, seminiferous tubule degeneration
Aldrin	309-00-2	Liver	Hepatotoxicity
Ammonia	7664-41-7	Sensory	Decreased taste threshold
Anthracene	120-12-7	--	No observed effects
Antimony	7440-36-0	Blood	Blood glucose and cholesterol, decreased longevity
Aroclor 1016	12674-11-2	Reproductive system	Decreased birth weights
Aroclor 1254	11097-69-1	Eye	Ocular exudate, inflamed and prominent meibomian glands
		General toxicity	Distorted growth of fingers and toenails
		Immune system	Decreased amtibody (IgM and IgG) response to sheep erythrocytes
Arsenic, inorganic	7440-38-2	Skin	Hyperpigmentation, keratosis, and possible vascular complications
Barium	7440-39-3	Blood pressure	Increased blood pressure
Benzaldehyde	100-52-7	Gastrointestinal	Forestomach lesions
		Kidney	Kidney toxicity
Benzidine	92-87-5	Liver	Liver cell alterations in females
		Nervous system	Brain cell vacuolization
Benzoic acid	65-85-0	--	No observed effects
Beryllium	7440-41-7	--	No adverse effects observed
Biphenyl, 1,1-	92-52-4	Kidney	Kidney damage
bis(2-Ethylhexyl)phthalate	117-81-7	Liver	Increased relative liver weight
bis(Chloromethyl)ether	542-88-1	--	No observed effects
Bromodichloromethane	75-27-4	Kidney	Renal cytomegaly
Bromoform	75-25-2	Liver	Hepatic lesions
Butyl benzyl phthalate	85-68-7	Liver	Significantly increased liver-to-body weight and liver-to-brain weight ratios
Cadmium	7440-43-9	Kidney	Significant proteinuria
Carbon disulfide	75-15-0	Reproductive	Fetal toxicity and malformations
Chlordane	57-74-9	Liver	Hepatocyte regeneration
Chlorine	7782-50-5	--	No observed effects

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TABLE A-2 (Continued)

TARGET ORGANS AND CRITICAL EFFECTS
FOR COMPOUNDS WITH REFERENCE DOSE VALUES

(Page 2 of 8)

Compound	CAS No.	Target Organ	Critical Effect
Chloroaniline, 4-	106-47-8	Spleen	Nonneoplastic lesions of the splenic capsule
Chlorobenzene	108-90-7	Liver	Histopathologic changes in liver
Chlorobenzilate	510-15-6	Gastrointestinal	Decreased stool quantity, food consumption, and body weight
		Nervous system	Hyperirritability
Chloroform	67-66-3	Liver	Fatty cyst formation in liver
Chloronaphthalene, 2-	91-58-7	Respiratory	Dyspnea, abnormal appearance, liver enlargement
Chlorophenol, 2-	95-57-8	Reproductive	Reproductive effects
Chlorotoluene, o-	95-49-8	Body weight	Decrease in body weight gain
Chlorpyrifos	2921-88-2	Blood	Decreased plasma cholinesterase activity
Chromium	7440-47-3	--	No observed effects
Chromium VI	18540-29-9	--	No observed effects
Cresol, o-(2-methylphenol)	95-48-7	Body weight	Decreased body weights
		Nervous system	Neurotoxicity
Cresol, p-	106-44-5	Whole body	Maternal death
		Nervous system	Hypoactivity
		Respiratory	Respiratory distress
Cumene	98-82-8	Kidney	Increased average kidney weight
Cyanide	57-12-5	--	No observed effects
Cyanogen	460-19-5	Body weight	Weight loss
		Nervous system	Myelin degeneration
		Thyroid	Thyroid effects
Cyanogen bromide	506-68-3	Body weight	Weight loss
		Nervous system	Myelin degeneration
		Thyroid	Thyroid effects
Cyanogen chloride	506-77-4	Body weight	Weight loss
		Neutroxicity	Myelin degeneration
		Thyroid	Thyroid effects
DDT, 4,4'-	50-29-3	Liver	Liver lesions
Demeton	8065-48-3	Nervous system	Cholinesterase inhibition
		Eye	Optic nerve degeneration
Diazinon	333-41-5	Blood	Decreased cholinesterase activity
Dibromochloromethane	124-48-1	Liver	Hepatic lesions
Dibromoethane, 1,2-	106-93-4	Reproductive system	Spermatogenic effects
Dibutyl phthalate	84-74-2	Death	Increased mortality
Dichlorobenzene, o-	95-50-1	--	No adverse effects observed
Dichlorodifluoromethane (CFC-12)	75-71-8	Body weight	Reduced body weight

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TABLE A-2 (Continued)

TARGET ORGANS AND CRITICAL EFFECTS
FOR COMPOUNDS WITH REFERENCE DOSE VALUES

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Compound	CAS No.	Target Organ	Critical Effect
Dichloroethane, 1,1-	75-34-3	--	No observed adverse effects (route-to-route extrapolation)
Dichloroethene, 1,1-	75-35-4	Liver	Hepatic lesions
Dichloroethene, trans-1,2-	156-60-5	Blood	Increased serum alkaline phosphatase in male mice
Dichloroethylene, cis-1,2-	156-59-2	Organ weight	Increased organ weight
		Respiratory	hypertrophy/hyperplasia of the nasal respiratory epithelium
Dichlorophenol, 2,4-	120-83-2	Immunotoxicity	Decreased delayed hypersensitivity response
Dichlorophenoxyacetic acid, 2,4- (2,4-D acid)	94-75-7	Blood	Hematologic toxicity
		Kidney	Hepatic toxicity
		Liver	Renal toxicity
Dichloropropene, 1,3-	542-75-6	Organ weights	Increased organ weights
Dichlorvos	62-73-7	Nervous system	Brain cholinesterase inhibition
		Blood	Plasma red blood cell cholinesterase inhibition
Dieldrin	60-57-1	Liver	Liver lesions
Diethyl phthalate	84-66-2	Body weight	Decreased growth rate and food consumption
		Organ weight	Altered organ weights
Dimethylphenol, 2,4-	105-67-9	General toxicity	Lethargy, prostration, ataxia,
		Blood	Hematological changes
Dimethylphthalate	131-11-3	Kidney	Kidney effects
Dinitrobenzene, 1,2-	528-29-0	Spleen	Increased spleen weight
Dinitrobenzene, 1,3-	99-65-0	Spleen	Increased spleen weight
Dinitrobenzene, 1,4-	100-25-4	Spleen	Increased spleen weight
Dinitro-o-cyclohexylphenol, 4,6-	131-89-5	Eye	Cataract formation
Dinitrophenol, 2,4-	51-28-5	Eye	Cataract formation
Dinitrotoluene, 2,4-	121-14-2	Gastrointestinal	Heinze bodies and biliary tract hyperplasia
		Nervous system	Neurotoxicity
Dinitrotoluene, 2,6-	606-20-2	Death	Decreased survival
		Blood	Heinze bodies, methemoglobinemia
		Gastrointestinal	Hyperplasia of the bile duct
		Kidney	Histopathologic changes in the kidney
		Nervous system	Neurotoxic effects
Di-n-octyl phthalate	117-84-0	Kidney	Increased kidney weight
		Liver	Increased liver weight; increased SGOT and SGPT activity
Diphenylamine	122-39-4	Body weight	Decreased body weight gain
		Kidney	Increased kidney weight
		Liver	Increased liver weights

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TABLE A-2 (Continued)

TARGET ORGANS AND CRITICAL EFFECTS
FOR COMPOUNDS WITH REFERENCE DOSE VALUES

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Compound	CAS No.	Target Organ	Critical Effect
Disulfoton	298-04-4	Eye	Optic nerve degeneration
		Nervous system	Cholinesterase inhibition
Endosulfan I	115-29-7	Body weight	Decrease in body weight gain
		Nervous system	Neurotoxicity
		Kidney	Marked progressive glomerulonephrosis and blood vessel anurysms in males
Endothall	145-73-3	Gastrointestinal	Increased absolute and relative weights of stomach and small intestine
Endrin	72-20-8	Nervous system	Occasional convulsions
		Liver	Mild histological lesions
Epichlorohydrin	106-89-8	Kidney	Kidney lesions (route-to-route extrapolation)
Ethoxyethanol, 2-	110-80-5	Body weight	Decreased body weight
Ethylbenzene	100-41-4	Kidney	Kidney toxicity
		Liver	Liver toxicity
Ethylene glycol	107-21-1	Kidney	Kidney toxicity
Ethylene thiourea	96-45-7	Thyroid	Increased incidence of thyroid hyperplasia
Ethylmethacrylate	97-63-2	Kidney	Increased relative weight of the kidney
Fluoranthene	206-44-0	Blood	Hematological alterations and clinical effects
		Kidney	Nephropathy
		Liver	Increased liver weights
Fluorene	86-73-7	Blood	Decreased red blood cell count, packed cell volume and hemoglobin
Formaldehyde	50-00-0	Body weight	Reduced weight gain, histopathology in rats
Formic acid	64-18-6	Body weight	Decreased growth rate
Freon 113	76-13-1	Nervous system	Psychomotor impairment
Furan	110-00-9	Liver	Hepatic lesions
Furfural	98-01-1	Liver	Mild hepatocellular vacuolization
Glycidaldehyde	765-34-4	Adrenal	Enlarged adrenals
		Blood	Hydropic renal pelvis and hematopoietic effects
		Body weight	Retarded weight gain
Heptachlor	76-44-8	Liver	Liver weight increases in males only
Heptachlor epoxide	1024-57-3	Liver	Increased liver-to-body weight ratio
Hexachlorobenzene	118-74-1	Liver	Liver effects
Hexachlorobutadiene	87-68-3	Kidney	Renal tubules regeneration
Hexachlorocyclopentadiene	77-47-4	Gastrointestinal	Stomach lesions
Hexachloroethane	67-72-1	Kidney	Atrophy and degeneration of renal tubules

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TABLE A-2 (Continued)

TARGET ORGANS AND CRITICAL EFFECTS
FOR COMPOUNDS WITH REFERENCE DOSE VALUES

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Compound	CAS No.	Target Organ	Critical Effect
Hexachlorophene	70-30-4	Salivary gland	Swollen
		Brain and optic nerve	Status spongiosis
Hexane, n-	110-54-3	Nervous system	Neuropathy
		Respiratory	Epithilial lesions in the nasal cavity
Isophorone	78-59-1	Kidney	Kidney pathology
Malathione	121-75-5	Blood	Red blood cell cholinesterase depression
Maleic hydrazide	123-33-1	Kidney	Renal dysfunction
Malononitrile	109-77-3	Liver	Liver effects
		Spleen	Spleen effects
Manganese	7439-96-5	Nervous system	Central nervous system effects
Mercuric chloride	7787-94-7	Immune system	Autoimmune effects
Mercury (inorganic)	7439-97-6	Nervous system	Neurotoxicity
Merphos	150-50-5	Nervous system	Ataxia and delayed neurotoxicity
		Wholebody	Decreased body weight
Methacrylonitrile	126-98-7	Liver	Increased SGOT and SGPT levels
Methanol	67-56-1	Nervous system	Brain cholinesterase inhibition
		Blood	Plasma red blood cell cholinesterase inhibition
Methoxychlor	72-43-5	Reproductive	Excessive loss of litter
Methoxyethanol, 2-	109-86-4	Reproductive	Testicular effects (route-to-route extrapolation)
Methyl acetate	79-20-9	Liver	Increased alkaline phosphatase and increased SGPT
Methyl bromide	74-83-9	Gastrointestinal	Epithelial hyperplasia of the forestomach
Methyl ethyl ketone	78-93-3	Reproductive	Decreased fetal birth weight
Methyl isobutyl ketone	108-10-1	Kidney	Increased urinary protein
		Liver	Increased absolute and relative weights of the liver
		Nervous system	Lethargy
Methyl mercury	22967-92-6	Nervous system	Developmental neurological abnormalities in human infants
Methyl parathion	298-00-0	Blood	Red blood cell cholinesterase inhibition, reduced hemoglobin, hematocrit and red blood cells
Methyl styrene (mixed isomers)	25013-15-4	Respiratory	Nasal cavity lesions (route-to-route extrapolation)
Methylene bromide	74-95-3	Blood	Increased carboxyhemoglobin (route-to-route extrapolation)
Methylene chloride	75-09-2	Liver	Liver toxicity
Methylphenol, 3-(m-Cresol)	108-39-4	Body weight	Decreased body weights
		Nervous system	Neurotoxicity
Naled	300-76-5	Nervous system	Brain cholinesterase inhibition
Nickel, soluble salts	7440-02-0	Body weight	Decreased body weight
		Organ weight	Decreased organ weights
Nitroaniline, 2-	88-74-4	Blood	Hematological effects

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TABLE A-2 (Continued)

TARGET ORGANS AND CRITICAL EFFECTS
FOR COMPOUNDS WITH REFERENCE DOSE VALUES

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Compound	CAS No.	Target Organ	Critical Effect
Nitrobenzene	98-95-3	Adrenal	Adrenal lesions
		Blood	Hemolytic anemia
		Liver	Renal lesions
		Renal	Hepatic lesions
N-nitrosodi-*n*-propylamine	621-64-7	--	No observed adverse effects
Pentachlorobenzene	608-93-5	Kidney	Kidney toxicity
		Liver	Liver toxicity
Pentachloronitrobenzene	82-68-8	Liver	Hepatotoxicity
Pentachlorophenol	87-86-5	Kidney	Kidney pathology
		Liver	Liver pathology
Phenol	108-95-2	Reproductive	Reduced fetal body weight in rats
Phorate	298-02-2	Nervous system	Cholinesterase inhibition
Phthalic anhydride	85-44-9	Kidney	Histopathology
		Respiratory	Lung damage
Pronamide	23950-58-5	--	No observed effects
Propargyl alcohol	107-19-7	Kidney	Hepatotoxicity
		Liver	Renal toxicity
Propylene glycol monomethyl ether	107-98-2	Kidney	Histopathologic changes of the kidney
		Liver	Histopathologic changes of the liver
Pyrene	129-00-0	Kidney	Renal tubular pathology and decreased kidney weights
Pyridine	110-86-1	Liver	Increased liver weight
Ronnel	299-84-3	Liver	Liver effects
Selenium	7782-49-2	Respiratory	Clinical selenosis
Silver	7440-22-4	Skin	Argyria
Strychnine and salts	57-24-9	General	Toxicity and histopathology
Styrene	100-42-5	Blood	Red blood cell effects
		Liver	Liver effects
Tetrachlorobenzene, 1,2,4,5-	95-94-3	Kidney	Kidney lesions
Tetrachloroethane (carbon tetrachloride)	56-23-5	Liver	Liver lesions
Tetrachloroethane, 1,1,1,2-	630-20-6	Kidney	Mineralization of the kidneys in males
		Liver	Hepatic clear cell changes in females
Tetrachloroethene	127-18-4	Liver	Hepatotoxicity in mice, weight gain in rats
Tetrachlorophenol, 2,3,4,6-	58-90-2	Liver	Increased liver weight and centrilobular hypertrophy
Thallium	7440-28-0	Liver	Increased levels of SGOT and LDH
Toluene	108-88-3	Kidney	Changes in kidney weights
		Liver	Changes in liver weights

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TABLE A-2 (Continued)

TARGET ORGANS AND CRITICAL EFFECTS
FOR COMPOUNDS WITH REFERENCE DOSE VALUES

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Compound	CAS No.	Target Organ	Critical Effect
Toluene-2,6-diamine	823-40-5	--	No adverse effects observed
Trichlorobenzene, 1,2,4-	120-82-1	Adrenal	Increased adrenal weights; vacuolation of zona fasciculate in the cortex
Trichloroethane, 1,1,2-	79-00-5	Blood	Clinical serum chemistry
Trichlorofluoramethane (Freon 11)	75-69-4	Death	Decreased survival
		General	Histopathology
Trichlorophenol, 2,4,5-	95-95-4	Kidney	Kidney pathology
		Liver	Liver pathology
Trichloropropane, 1,2,3-	96-18-4	Blood	Alterations in clinical chemistry and reduction in red cell mass
Trinitrobenzene, sym-	99-35-4	Spleen	Increased spleen weight
Trinitrotoluene, 2,4,6-	118-96-7	Liver	Liver effects
Vinyl acetate	108-05-4	Body weight	Decreased body weight
		Kidney	Altered kidney weight
Xylenes	1330-20-7	Death	Increased mortality
		Body weight	Decreased body weight
		Nervous system	Hyperactivity
Xylene, m-	108-38-3	Death	Increase mortality
		Body weight	Decreased body weight
		Nervous system	Hyperactivity
Xylene, o-	95-47-6	Nervous system	Hyperactivity
Zinc	7440-66-6	Blood	47% decrease in erythrocyte superoxide dismutase concentration in females

Note:

Target organ and critical effect information presented in this table is intended only to provide the information needed to break down calculated hazard quotients for various chemicals, based on the target organs that they affect (see Section 7.3 of the HHRAP). The information is intended to be neither (1) an exhaustive list of the potential toxic effects of a compound, or (2) an indication that toxicological studies for a substance are inadequate because the target organ or critical effect for each particular substance is limited to one or two reported health effects. The noncancer reference dose (RfD) for ingestion exposure, or the reference concentration (RfC) for inhalation exposures, is generally based on the experimental dose that produces no adverse effects in the most sensitive laboratory animal tested (referred to as the no-observed-adverse effects-level [NOAEL]). If all of the doses used in experimental studies produce some effect, the lowest dose at which an adverse effect is observed (referred to as the lowest-observed-adverse-effect-level) is used to determine the RfD or RfC. Both uncertainty factors and modifying factors are included in the calculation of RfDs to ensure that these values are protective of human health (see Appendix A-3) (U.S. EPA 1988).

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References:

U.S. Environmental Protection Agency (EPA) 1988. *Background Document—RfD Description and Use in Health Risk Assessments*.

U.S.EPA. 1995. "Health Effects Assessment Summary Tables."Fiscal Year-1995 Annual. Office of Solid Waste and Emergency Response. Washington, D.C. EPA/540/R-95/036. May.

U.S.EPA. 1997. Intergrated Risk Information System. December.

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APPENDIX A-3

COMPOUND SPECIFIC PARAMETER VALUES

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APPENDIX A-3
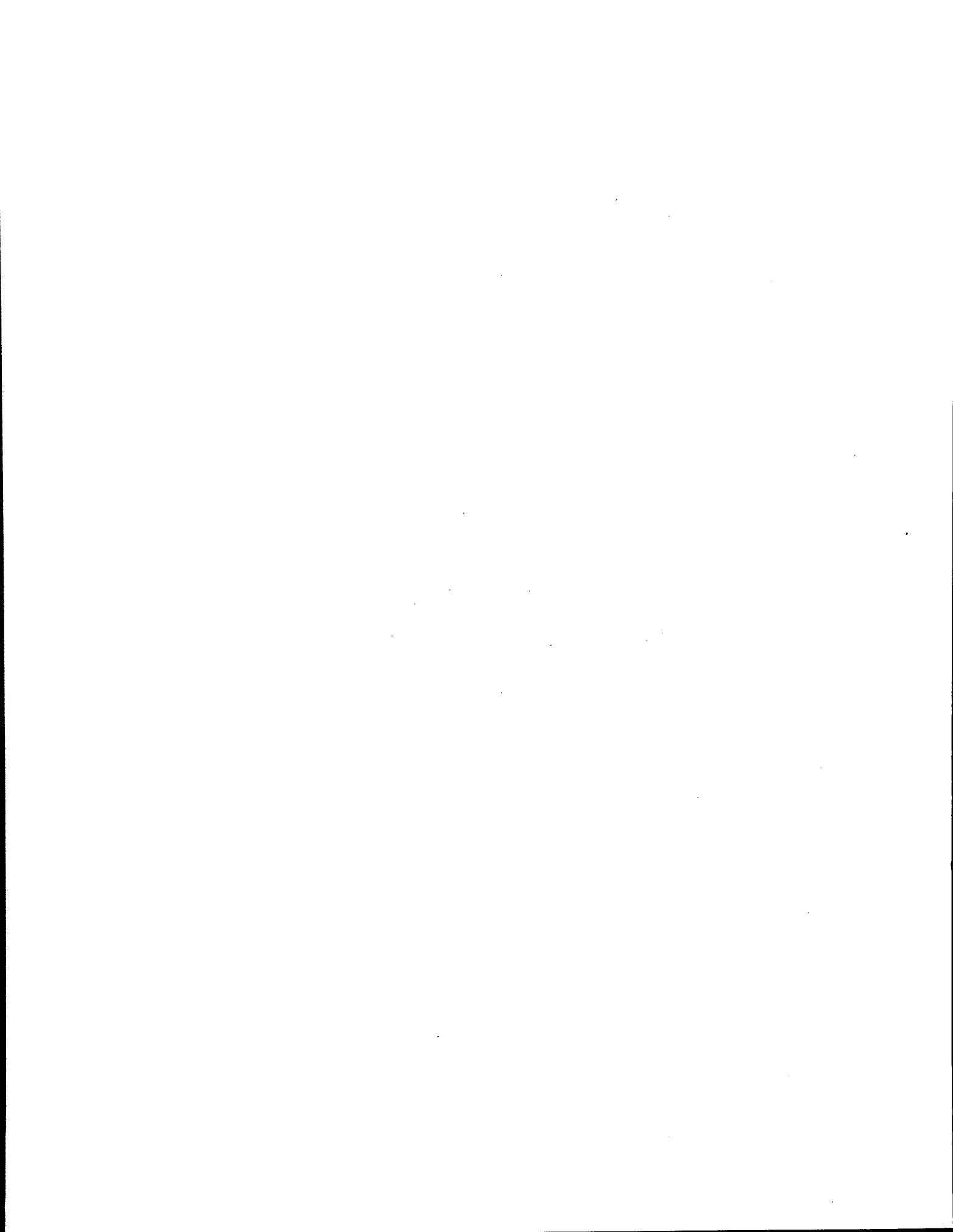
LIST OF VARIABLES AND COMPOUND-SPECIFIC PARAMETERS

ρ_{air} = Density of air (g/cm^3)

ρ_{forage} = Density of forage (g/cm^3)

Ba_{beef} = Biotransfer factor in beef
(mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)

$Ba_{chicken}$ = Biotransfer factor in chicken
(mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)

Ba_{egg} = Biotransfer factor in eggs
(mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)

Ba_{milk} = Biotransfer factor in milk
(mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)

Ba_{pork} = Biotransfer factor in pork
(mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)

BAF_{fish} = Bioaccumulation factor in fish
(mg COPC/kg FW tissue)/(mg COPC/L total water column)
OR (L water/kg FW tissue)

BCF_{fish} = Bioconcentration factor in fish (L/kg FW OR unitless)

Br_{ag} = Plant-soil bioconcentration factor in aboveground produce
(µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless

$Br_{forage/silage}$ = Plant-soil bioconcentration factor in forage and silage
(µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless

Br_{grain} = Plant-soil bioconcentration factor in grain
(µg COPC/g DW grain)/(µg COPC/g DW soil)—unitless

$Br_{rootveg}$ = Plant-soil bioconcentration factor for belowground produce
(µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless

$BSAF_{fish}$ = Biota-sediment accumulation factor in fish
(mg COPC/kg lipid tissue)/(mg COPC/kg sediment)—unitless

B_{vol} = Volumetric air-to-leaf biotransfer factor in leaf
(µg COPC/L FW plant)/(µg COPC/L air)—unitless

Bv_{ag} = COPC air-to-plant biotransfer factor for aboveground produce
(µg COPC/g DW plant)/(µg COPC/g air)—unitless

$Bv_{forage/silage}$ = Air-to-plant biotransfer factor in forage and silage
(µg COPC/g DW plant)/(µg COPC/g air)—unitless

c = Junge constant = 1.7 x 10^{-04} (atm-cm)

D_a = Diffusivity of COPC in air (cm^2/s)

D_w = Diffusivity of COPC in water (cm^2/s)

$f_{oc,bs}$ = Fraction of organic carbon in bottom sediment (unitless)

$f_{oc,s}$ = Fraction of organic carbon in soil (unitless)

$f_{oc,sw}$ = Fraction of organic carbon in suspended sediment (unitless)

f_{water} = Fraction of COPC in water (unitless)

F_v = Fraction of COPC air concentration in vapor phase (unitless)

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Fw	=	Fraction of wet deposition that adheres to plant surfaces (unitless)
H	=	Henry's law constant
Inhalation CSF	=	Inhalation cancer slope factor $(mg/kg\text{-}day)^{-1}$
Inhalation URF	=	Inhalation unit risk factor $(\mu g/m^3)^{-1}$
Kd_s	=	Soil-water partition coefficient (mL water/g soil OR cm^3 water/g soil)
Kd_{sw}	=	Suspended sediment-surface water partition coefficient (L water/kg suspended sediment OR cm^3 water/g suspended sediment)
Kd_{bs}	=	Bed sediment-sediment pore water partition coefficient (L water/kg bottom sediment OR cm^3 water/g bottom sediment)
K_{ow}	=	Octanol/water partitioning coefficient (mg COPC/L octanol)/(mg COPC/L octanol)—unitless
K_{oc}	=	Soil organic carbon-water partition coefficient (mL water/g soil)
ksg	=	COPC soil loss constant due to biotic and abiotic degradation (yr^{-1})
MW	=	Molecular weight of COPC (g/mole)
$p_L^{\bullet}$	=	Liquidphase vapor pressure of COPC (atm)
$p_s^{\bullet}$	=	Solid-phase vapor pressure of COPC (atm)
Oral CSF	=	Oral cancer slope factor $(mg/kg\text{-}day)^{-1}$
R	=	Universal gas constant $(atm\text{-}m^3/mol\text{-}K)$
RCF	=	Root concentration factor (μg COPC/g DW plant)/(μg COPC/mL soil water)
RfC	=	Reference concentration (mg/m^3)
RfD	=	Reference dose (mg/kg/day)
Rp	=	Interception factor of edible portion of plant (unitless)
S	=	Solubility of COPC in water (mg COPC/L water)
ΔS_f	=	Entropy of fusion $[\Delta S_f/R = 6.79$ (unitless)]
S_T	=	Whitby's average surface area of particulates (aerosols) $= 3.5 \times 10^{-06} \ cm^2/cm^3$ air for background plus local sources $= 1.1 \times 10^{-05} \ cm^2/cm^3$ air for urban sources
$t_{1/2}$	=	Half-time of COPC in soil (days)
T_a	=	Ambient air temperature (K)
T_m	=	Melting point temperature (K)
TEF	=	Toxicity equivalency factor (unitless)
Vp	=	Vapor pressure of COPC (atm)

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APPENDIX A-3

The following sections provide the methodology and rationale followed for the selection or development of compound-specific parameter values recommended by U.S. EPA OSW. Compound-specific values are provided for (1) physical and chemical properties, (2) fate-and-transport parameters, and (3) health benchmarks. A summary table of all compound-specific parameter values is provided at the end of this appendix, followed by individual parameter-value tables for each compound. The individual parameter-value tables cite sources for each parameter value.

A3.1   PRIMARY GUIDANCE DOCUMENTS

Throughout Appendix A-3, the following guidance documents are referenced as the primary sources for the development and comparision of compound-specific parameter values, and used to the fullest extent possible to provide consistency. Therefore, in this appendix, the term **primary guidance documents** refers to the following documents:

- U.S. EPA. 1994f. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes: Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* Office of Emergency and Remedial Response (OERR). Office of Solid Waste. December 14.

- U.S. EPA. 1995b. *Review Draft Development of Human Health Based and Ecologically Based Exit Criteria for the Hazardous Waste Identification Project.* Volumes I and II. Office of Solid Waste. March 3.

- North Carolina Department of Environment, Health, and Natural Resources (NC DEHNR). 1997. *North Carolina Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

To ensure consistency, sources referenced in the primary guidance documents were also evaluated. Information for certain compounds like PCDDs, PCDFs, and mercury were obtained from the following documents:

- U.S. EPA. 1994a. *Estimating Exposure to Dioxin-Like Compounds.* External Review Draft Report. Volumes I-III. Office of Research and Development. Washington, DC. EPA/600/6-88/005Ca,b,c.

- U.S. EPA. 1997g. *Mercury Study Report to Congress. Volume III: Fate and Transport of Mercury in the Environment.* Office of Air Quality Planning and Standards and Office of Research and Development. EPA-452/R-97-005. December.

U.S. EPA (1994a) provides various parameter values for (but are not limited to) PCDDs, PCDFs, and PCBs. U.S. EPA (1997g) provides various parameter values for mercuric compounds including elemental mercury, mercuric chloride, and methyl mercury.

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A3.2   GENERAL ANALYSIS AND METHODOLOGY

This section describes the general analysis and methodology followed for the development of compound-specific parameter values presented. Compound-specific parameter values in the primary guidance documents and other sources generally were evaluated as follows:

1. Compound-specific values for each parameter were compared among the primary guidance documents and the following observations were noted:

    a. Parameter values provided in U.S. EPA (1994f) are limited to 24 compounds. For these compounds, sources were referenced specifically to each parameter, in addition to the methodology used to obtain the respective values.

    b. U.S. EPA (1995b) provides various parameter values for a comprehensive list of compounds. The methodology used for determining values was covered in detail. However, parameter values for each compound were not referenced to a specific source. Although a comprehensive list of sources was provided, it is difficult to determine which parameter value for a compound was obtained from which source.

    c. NC DEHNR (1997) provides various parameter values for a comprehensive list of compounds, including congeners of polychlorinated dibenzo(p)dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs). However, the sections citing the methodology and sources of values in the NC DEHNR (1997) were reproduced directly from U.S. EPA (1994f). Therefore, in NC DEHNR (1997), the compound-specific parameter values that were provided did not correlate with the sections citing the methodology and sources of values. In addition, only a partial list of sources was provided for the values. Therefore, it was not possible to determine the actual source of values with certainty.

2. Sources of values referenced in the primary guidance documents were further researched and evaluated. Observations affecting usability are included in parameter-specific discussions for each compound, as appropriate.

3. Values provided in the primary guidance documents were used only when the sources and applicability of such values could be verified. Additional sources of parameter values were evaluated, used, and referenced when technically justified.

4. Recommended parameter values obtained using correlations or equations were calculated using the recommended values for these variables provided in this HHRAP.

In general, for the selection of parameter values, the following three steps were followed:

1. Whenever measured parameter values were available in published literature studies, they were preferred for use over other types of data. When multiple measured values were available, the geometric mean of the parameter values is recommended for use.

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2.   In the absence of measured values in published literature that could not be directly evaluated, parameter values compiled or adopted for use by the primary guidance documents, U.S. EPA (1994a), and U.S. EPA (1997g) are recommended.

3.   If unable to obtain acceptable values from published literature or the primary guidance documents, parameter values were estimated or calculated using correlation equations based on sound scientific judgment.

The following sections, A3.3 through A3.5, provide compound-specific parameter values, which are categorized and discussed as follows: (1) organic compounds, including polychlorinated biphenyls (PCB), and excluding methyl mercury, PCDDs and PCDFs, (2) PCDDs and PCDFs, (3) all metals except mercury, and (4) the mercuric compounds—mercury (elemental; metal), mercuric chloride (divalent inorganic mercury), and methyl mercury (organic mercury).

For each of the parameters, the sources of values referenced in this HHRAP are followed by a discussion and justification of their selection. There is also a brief discussion of the methodology followed by each of the primary guidance documents. This provides a complete evaluation and comparison of the compound-specific parameter values provided in the primary guidance documents that are currently used to conduct risk assessments.

A3.3   PHYSICAL AND CHEMICAL PROPERTIES

A3.3.1   Molecular Weight (*MW*)

Molecular weight (*MW*) of a compound is defined as the sum of atomic weights of all atoms in the compound's molecule.

Organics and Metals For most organics (except PCDDs and PCDFs) and metals, this HHRAP provides *MW* values that were obtained from the following:

•   Budavari, S., M.J. O'Neil, A. Smith, and P.E. Heckelman. 1989. *The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals.* 11th Edition. Merck and Company, Inc. Rahway, New Jersey.

MW values not provided in Budavari, O'Neil, Smith, and Heckelman (1989) were obtained from the following document:

•   Montgomery, J.H., and L.M. Welkom. 1991. *Groundwater Chemicals Desk Reference.* Lewis Publishers. Chelsea, Michigan.

Because Budavari, O'neil, Smith, and Heckelman (1989) provides *MW* values for most of the compounds evaluated, it was used as the primary source to ensure consistency. *MW* values are based on the compound's formula; and, the values in Budavari, O'Neil, Smith, and Heckelman (1989) are the same as the values cited in several literature sources. *MW* values for most of the compounds in the primary guidance documents were also obtained from Budavari, O'Neil, Smith, and Heckelman (1989).

PCDDs and PCDFs *MW* values for PCDDs and PCDFs were obtained from U.S. EPA (1994a).

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Mercuric Compounds MW values for mercury and mercuric chloride were obtained from Budavari and others (1989). MW value for methyl mercury was obtained from U.S. EPA (1997g).

A3.3.2   Melting Point Temperature (T_m)

Melting point temperature (T_m) is the temperature of the compound (in degree Kelvin [K]) at which the solid state of the compound undergoes a phase change to a liquid phase. At ambient temperatures and at an atmpospheric pressure of 1 atmosphere, compounds are either in a solid or liquid state. The compound liquid or solid state is provided in the summary tables of compound-specific parameter values.

Organics and Metals For most organics (except PCDDs and PCDFs) and metals, this HHRAP provides values for T_m that were obtained from Budavari, O'Neil, Smith, and Heckelman (1989). T_m values not provided in Budavari, O'Neil, Smith, and Heckelman (1989) were obtained from Montgomery and Welkolm (1991).

Because Budavari, O'Neil, Smith, and Heckelman (1989) provides T_m values for most of the compounds evaluated, it was used as the primary source to ensure consistency. T_m values in Budavari, O'Neil, Smith, and Heckelman (1989) were generally within 2 to 3 degrees of the values provided in literature sources reviewed. T_m values for most compounds in the primary guidance documents were also obtained from Budavari, O'Neil, Smith, and Heckelman (1989).

PCDDs and PCDFs Tm values for PCDDs and PCDFs were obtained from U.S. EPA (1994a). U.S. EPA (1994a) provides T_m values for PCDDs and PCDFs, that were obtained from various literature sources.

A3.3.3   Vapor Pressure (Vp) and Aqueous Solubility (S)

The vapor pressure (Vp) of a substance is defined as the pressure in atmospheres exerted by the vapor (gas) of a compound when it is under equilibrium conditions. It provides a semi-quantitative rate at which it will volatilize from soil and/or water. The aqueous solubility (S) of a compound is defined as the saturated concentration of the compound in water (mg COPC/L water) at a given temperature and pressure, usually at soil/water temperatures and atmospheric pressure (Montgomery and Welkom 1991).

Organics For most organics (except PCDDs and PCDFs), values for Vp and S were obtained from the following:

- U.S. EPA 1994c. *Draft Report Chemical Properties for Soil Screening Levels.* Prepared for the Office of Emergency and Remedial Response. Washington, DC. July 26.

U.S. EPA (1994c) provides measured, calculated, and estimated values for Vp and S that were obtained from various literature sources. Vp values in U.S. EPA (1994c) were generally either measured (at 20°C to 25°C) or calculated values obtained from various literature sources. U.S. EPA (1994c), however, provides values for Vp corrected to 25°C. U.S. EPA (1995b) states that, because the distribution of many of the parameters is skewed, the geometric mean or the median values were preferable to the arithmetic mean values. Therefore, when available geometric mean values were preferred over the arithmetic mean values. The geometric mean of the temperature corrected Vp values, determined from measured and calculated values, is recommended for use in this HHRAP.

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In U.S. EPA (1994c), S values were either measured (at 20°C to 30°C) or calculated values obtained from various literature sources. The geometric mean S value, calculated from measured and calculated values, is recommended for use in this HHRAP. Although S values were measured at temperatures ranging from 20°C to 30°C, U.S. EPA (1994c) states that S values were not corrected to 25°C, because the variability in solubilities measured at 20°C to 25°C was within the overall range of measured values.

U.S. EPA (1994c) is the preferred source, because (1) sources and the conditions at which each value was obtained are provided, and (2) values were provided to 2 significant figures. Also, U.S. EPA (1994c) provides multiple Vp and S values for each compound from several different literature sources; providing a recent, more comprehensive compilation of reported literature values. Vp and S values from U.S. EPA (1994c) were generally consistent with those provided in U.S. EPA (1994f), U.S. EPA (1995b), and NC DEHNR (1997).

When Vp and S values were not available in U.S. EPA (1994c), they were obtained from one of three sources, in the following order of preference:

1.   U.S. EPA (1994f)

2.   U.S. EPA (1995b); values from which were obtained from one of three sources:

   a.   Mackay, D., W.Y. Shiu, and K.C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental fate for Organic Chemicals. Volume I - Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Volume II-Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins and Dibenzofurans. Volume III - Volatile Organic Chemicals.* Lewis Publishers. Boca Raton, Florida.

   b.   Howard, P.H. 1989-1993. *Handbook of Environmental Fate and Exposure Data For Organic Chemicals. Volumes I: Large Production and Priority Pollutants (1989). Volume II: Solvents (1990). Volume III: Pesticides (1991). Volume IV: Solvents2 (1993).* Lewis Publishers. Chelsea, Michigan.

   c.   Other referenced literature sources, when values were not available in Mackay, Shiu, and Ma (1992) or Howard (1989-1993).

3.   U.S. EPA. 1994b. *Superfund Chemical Data Matrix (SCDM).* Office of Emergency and Remedial Response. Washington, DC. June.

Vp and S values in U.S. EPA (1994f) were geometric mean values obtained from various literature sources. References specific to sources of values for each compound were provided in U.S. EPA (1994f) and were, therefore, preferred over U.S. EPA (1995b) values.

Most Vp and S values in U.S. EPA (1995b) were obtained from Mackay, Shiu, and Ma (1992) or Howard (1989-1993). Mackay, Shiu, and Ma (1992) and Howard (1989-1993) obtain the "best" values after evaluation of various literature sources.

Vp values in U.S. EPA (1994b) were obtained from various literature sources. S values in U.S. EPA (1994b) were the geometric mean of values obtained from various literature sources.

PCDDs and PCDFs *Vp* and *S* values for PCDDs and PCDFs were obtained from U.S. EPA (1994a). *Vp* and *S* values were either (1) measured, or (2) estimated by using the homologue (compound class with the same amount of chlorination) average method.

> **NOTE:** The phase—solid or liquid—of *Vp* values for all organics, including PCDDs and PCDFs, was indicated. This is based on whether the compound is in the solid or liquid phase at ambient soil temperatures.

Metals As cited in the primary guidance documents and in the literature, metals—except mercury—are considered (1) nonvolatile at ambient temperatures, and (2) insoluble in water, except as certain weak acids. Therefore, *Vp* and *S* values were not available for all metals (except mercury) in any of the literature sources reviewed.

Mercuric Compounds Mercury is a relatively volatile compound. *Vp* and *S* values for elemental mercury were obtained from Budavari, O'Neil, Smith, and Heckelman (1989); and are comparable to the values in the primary guidance documents. *Vp* and *S* values for mercuric chloride were obtained from U.S. EPA (1997g) and Budavari, O'Neil, Smith, and Heckelman (1989), respectively. *Vp* and *S* values for methyl mercury were not found in the literature.

A3.3.4   Henry's Law Constant (*H*)

Henry's Law constant (*H*) is also referred to as the air-water partition coefficient, and is defined as the ratio of the partial pressure of a compound in air to the concentration of the compound in water at a given temperature under equilibrium conditions. Henry's Law constant values generally can be (1) calculated from the theoretical equation defining the constant, (2) measured, or (3) estimated from the compound structure. Experimental and estimated *H* values from literature reports, however, are (1) very temperature-dependent and difficult to measure, (2) generally obtained from various literature sources that use different experimental and estimation methods, and (3) available for only a limited number of compounds.

Organics For organics (excluding PCDDs and PCDFs), *H* values were calculated from the following theoretical equation (Lyman, Reehl, and Rosenblast 1982) for consistency, using recommended *MW, S,* and *Vp* values provided in this HHRAP:

$$H = \frac{Vp \cdot MW}{S} \qquad\qquad \text{Equation A3-1}$$

$$
\begin{aligned}
H \;\; &= \;\; \text{Henry's Law constant (atm-m}^3\text{/mole)} \\
Vp \;\; &= \;\; \text{Vapor pressure of COPC (atm)} \\
S \;\; &= \;\; \text{Solubility of COPC in water (mg COPC/L water)}
\end{aligned}
$$

The primary guidance documents also used theoretical Equation A-3-1 to calculate *H* values.

PCDDs and PCDFs *H* values for PCDDs and PCDFs are calculated values obtained from U.S. EPA (1994a).

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Metals For all metals (except mercury), H is zero, because Vp—because of the nonvolatile nature of the metals—and S are assumed to be zero.

Mercuric Compounds H values for elemental mercury, mercuric chloride, and methyl mercury were obtained from U.S. EPA (1997g).

A3.3.5   Diffusivity of COPCs in Air (D_a) and Water (D_w)

Diffusivity or diffusion coefficients in air (D_a) and water (D_w) are used to calculate the liquid or gas phase transfer of a COPC into a waterbody.

Organics For organics (except PCDDs and PCDFs), diffusivity values were obtained directly from the CHEMDAT8 model chemical properties database (Worksheet DATATWO.WK1):

- U.S. EPA. 1994d. *CHEM8—Compound Properties Estimation and Data*. Version 1.00. CHEMDAT8 Air Emissions Program. Prepared for Chemicals and Petroleum Branch, OAQPS. Research Triangle Park. North Carolina. November 18.

The U.S. EPA (1994d) database uses empirical correlations with compound density and molecular weight to calculate diffusivity values. For compounds not in the U.S. EPA (1994d) database, diffusivity values were obtained by using the WATER8 model correlation equations for air and water diffusivities:

- U.S. EPA. 1995d. *WATER8—Air Emissions Models Wastewater Treatment*. Version 4.0. OAQPS. Research Triangle Park. North Carolina. May 1.

U.S. EPA(1995d) database values were predicted by using chemical-structural relationships. Diffusivity values for all compounds in the U.S. EPA (1994d) and (1995d) databases were either predicted or estimated. The primary guidance documents also recommended U.S. EPA (1994d) and (1995d) database model values. More recent documents, including the following, also recommended these values:

- U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document and User's Guide*. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

For diffusivity values that were not available in these databases, D_w and D_a values were calculated using the following equations cited and recommended for use in U.S. EPA (1997g):

$$D_{a,i} = \frac{1.9}{(MW_i)^{2/3}}$$

Equation A3-2a

$$D_{w,i} = \frac{22 \times 10^{-5}}{(MW_i)^{2/3}}$$

Equation A3-2b

U.S. EPA (1995b) recommended the use of standard default diffusivity values. U.S. EPA (1995b) stated that the diffusivity parameters vary slightly, and default values appear to be within the range of typical values. Values for diffusivity in air range from about 0.01 to 0.1 square centimeters per second (cm²/s);

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therefore, U.S. EPA (1995b) recommended a default value of 0.08 cm²/s. Values for diffusivity in water range from 1×10^{-06} to 1×10^{-05} cm²/s; therefore, U.S. EPA (1995b) recommended a default value of 8×10^{-06} cm²/s. Diffusivity values calculated using Equations A-3-2a and A-3-2b were within the range specified by U.S. EPA (1995b), and therefore, were adopted for use in this HHRAP.

PCDDs and PCDFs Diffusivity values in air and water for (1) 2,3,7,8-TCDD were obtained from U.S. EPA (1994e), and (2) 2,3,7,8-TCDF were obtained from U.S. EPA (1995d). For all other congeners of PCDDs and PCDFs, (1) a default *Dw* value of 8×10^{-06} cm²/s was used, and (2) *Da* values were calculated using the following equation recommended by U.S. EPA (1994a):

$$\frac{D_x}{D_y} = (\frac{MW_y}{MW_x})^{0.5}$$ Equation A3-2c

where

$\quad D_{x,y} \quad = \quad$ Diffusivities in air of compounds x and y (cm²/s)
$\quad MW_{x,y} \quad = \quad$ Molecular weights of compounds x and y (g/mol)

Da values for PCDD congeners were calculated by using the *Da* value and *MW* for 2,3,7,8-TCDD. *Da* values for PCDF congeners were calculated using the *Da* value and *MW* for 2,3,7,8-TCDF. This approach is consistent with the methodology specified in U.S. EPA (1994a).

Metals and Mercuric compounds For metals (except chromium and mercury), diffusivity values were not available in the literature. Diffusivity values for chromium and mercury were obtained from the U.S. EPA (1994d) database. Diffusivity values for mercuric chloride and methyl mercury were calculated using Equations A-3-2a and A-3-2b.

A3.3.6   Octanol/Water Partitioning Coefficient (K_{ow})

The *n*-octanol/water partitioning coefficient (K_{ow}) is defined as the ratio of the solute concentration in the water-saturated *n*-octanol phase to the solute concentration in the *n*-octanol-saturated water phase (Montgomery and Welkom 1991).

Organics For organics (except PCDDs and PCDFs), K_{ow} values were obtained from U.S. EPA (1994c). U.S. EPA (1994c) provides measured, calculated, and estimated K_{ow} values obtained from various literature sources. The geometric mean K_{ow} value, calculated from all measured and calculated values for each compound, is recommended in this HHRAP.

K_{ow} values that were not available in U.S. EPA (1994c) were obtained from one of three sources, in the following order of preference:

1.   U.S. EPA (1994f)

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2.   Karickhoff, S.W. and J.M. Long. 1995. "Internal Report on Summary of Measured, Calculated, and Recommended Log K_{ow} Values." Environmental Research Laboratory. Athens. April 10.

3.   U.S. EPA (1995b), values from which were obtained from one of three sources:

   a.   Mackay, D., W.Y. Shiu, and K.C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume I - Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Volume II - Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins and Dibenzofurans. Volume III - Volatile Organic Chemicals.* Lewis Publishers. Boca Raton, Florida.

   b.   Howard, P.H. 1989-1993. *Handbook of Environmental Fate and Exposure Data For Organic Chemicals. Volumes I: Large Production and Priority Pollutants (1989). Volume II: Solvents (1990). Volume III: Pesticides (1991). Volume IV: Solvents2 (1993).* Lewis Publishers. Chelsea, Michigan.

   c.   Other literature sources, when values were not available in Mackay, Shiu, and Ma (1992) and Howard (1989-1993).

U.S. EPA (1994c) is the preferred source of values because (1) sources were provided, (2) several literature values were provided, some of which are also cited by the primary guidance documents and Karickhoff and Long (1995), and (3) the values were provided to 2 significant figures.

U.S. EPA (1994f) is the second-choice source of K_{ow} values recommended; and provides geometric mean values obtained from various literature sources. Karickhoff and Long (1995) recommended arithmetic mean values obtained from various literature sources and was, therefore, preferred as the third-choice source of K_{ow} values when values were not available from the first two sources.

In order to reference specific sources of K_{ow} values for each compound, values from U.S. EPA (1995b) and NC DEHNR (1997) were used only when values were not available in the literature sources reviewed.

PCDDs and PCDFs K_{ow} values for the PCDDs and PCDFs were obtained from either U.S. EPA (1994a) or U.S. EPA (1992d). U.S. EPA (1994a) and U.S. EPA (1992d) provide K_{ow} values for PCDDs and PCDFs that were either measured values obtained from the literature or calculated by averaging the literature values within the homologue group. According to U.S. EPA (1994a), K_{ow} values for hexachlorodibenzofurans were not available in the literature. Therefore, as recommended in U.S. EPA (1994a), due to lack of data, homologue group average values for hexachlorodibenzodioxins were applied to hexachlorodibenzofurans.

Metals No K_{ow} values were available for metals, either in the literature or in the primary guidance documents. K_{ow} values for the metals were assumed to be zero, because the affinity of the metals to the octanol is almost zero.

Mercuric compounds No K_{ow} values were available in the literature for mercury and methyl mercury. For mercuric chloride, the K_{ow} value was obtained from U.S. EPA (1997g).

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A3.3.7   Soil Organic Carbon-Water Partition Coefficient (K_{oc})

The soil organic carbon-water partition coefficient (K_{oc}) or the organic carbon normalized soil sorption coefficient is defined as the ratio of adsorbed compound per unit weight of organic carbon to the aqueous solute concentration (Montgomery and Welkom 1991).

**Organics** Because of the soil mechanisms that are inherently involved, K_{oc} values for the ionizing organics and nonionizing organics are discussed separately.

A3.3.7.1   Ionizing Organic Compounds

Ionizing organic compounds include amines, carboxylic acids, and phenols. These compounds contain the functional groups that ionize under specific pH conditions, and include the following:

- Organic acids (2,4,6-trichlorophenol; pentachlorophenol; 2,3,4,5-tetrachlorophenol; 2,3,4,6-tetrachlorophenol; 2,4,5-trichlorophenol; 2,4-dichlorophenol; 2-chlorophenol; phenol; 2,4-dimethylphenol; 2-methylphenol; 2,4-dinitrophenol; and benzoic acid)

- Organic bases—n-nitroso-di-n-propylamine; n-nitrosodiphenylamine, and 4-chloroaniline)

K_{oc} values for ionizing organic compounds were obtained from U.S. EPA (1994c). U.S. EPA (1994c) provides K_{oc} values for the ionizing organic compounds that have been estimated on the basis of the degree of ionization and the relative proportions of neutral and ionized species. The primary guidance documents cite one value for the ionizing organics, independent of the pH. The primary guidance documents calculate K_{oc} values for the ionizing organics by using correlation equations containing K_{ow} that are applicable to nonionizing organics. However, K_{oc} values for ionizing compounds can vary vastly, depending on the pH conditions in the environment. Therefore, for the aforementioned ionizing organic compounds, this HHRAP prefers and provides estimated K_{oc} values that are based on pH.

K_{oc} values were estimated on the basis of the assumption that the sorption of ionizing organic compounds is similar to hydrophobic organic sorption, because the soil organic carbon is the dominant sorbent. According to U.S. EPA (1994c), for low pH conditions, these estimated values may overpredict sorption coefficients, because they ignore sorption to components other than organic carbon.

A3.3.7.2   Nonionizing Organic Compounds

Nonionizing organic compounds are all other organic compounds not listed earlier as ionizing. They include volatile organics, chlorinated pesticides, polynuclear aromatic hydrocarbons (PAHs), and phthalates. This HHRAP uses geometric mean of measured K_{oc} values provided in the following document:

- U.S. EPA. 1996b. _Soil Screening Guidance: Technical Background Document and User's Guide._ Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

U.S. EPA (1996b) calculated the geometric mean value from various measured values. For compounds for which K_{oc} values are not provided by U.S. EPA (1996b), K_{oc} values were calculated using K_{ow} correlation equations provided in the same document.

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NC DEHNR (1997) and U.S. EPA (1994f) use the following correlation equation to calculate K_{oc} from K_{ow} for all organics:

$$\log K_{oc} = 0.88\ (\log K_{ow}) + 0.114 \qquad (r^2 = 0.96)$$ Equation A-3-3

- Research Triangle Institute (RTI). 1992. *Preliminary Soil Action Level for Superfund Sites, Draft Interim Report.* Prepared for U.S. EPA Hazardous Site Control Division, Remedial Operations Guidance Branch. Arlington, Virginia. December.

However, according to U.S. EPA (1994c), the correlation between K_{oc} and K_{ow} can be improved considerably by performing separate linear regressions on two chemical groups. U.S. EPA (1994c) derives the following correlation equations from measured K_{oc} values cited in U.S. EPA (1994c) and U.S. EPA (1996b):

For phthalates and PAHs

$$\log K_{oc} = 0.97\ (\log K_{ow}) - 0.094 \qquad (r^2 = 0.99)$$ Equation A-3-4

For all organics except phthalates, PAHs, PCDDs, and PCDFs

$$\log K_{oc} = 0.78\ (\log K_{ow}) + 0.151 \qquad r^2 = 0.98$$ Equation A-3-5

Because of the improved regressions (r^2), U.S. EPA (1994c) recommended that correlation Equations A-3-4 and A-3-5 be used instead of correlation Equation A-3-3. U.S. EPA (1995b) also recommended that correlation Equations A-3-4 and A-3-5 be used.

Although U.S. EPA (1995b) recommended the use of correlation Equations A-3-4 and A-3-5, the following correlation equation was used by that document to calculate K_{oc} values for all organics except PCDDs and PCDFs:

$$\log K_{oc} = 0.983\ (\log K_{ow}) + 0.0002$$ Equation A-3-6

- DiToro, D.M., C.S. Zarba, D.J. Hansen, W.J. Berry, R.C. Swartz, C.E. Cowan, S.P. Pavlou, H.E. Allen, N.A. Thomas, and P.R. Paquin. 1991. "Technical Basis for Establishing Sediment Quality Criteria for Nonionic Compounds Using Equilibrium Partitioning." *Environmental Toxicology and Chemistry.* 10:1541-1583

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For the purposes of this HHRAP, values obtained by using correlation Equations A-3-3 through A-3-6, were compared. In general, more of the K_{oc} values obtained by using correlation Equations A-3-4 and A-3-5 were within the range of measured values in the literature than those obtained by using correlation Equations A-3-3 and A-3-6. Therefore, when measured K_{oc} values were not available, values were estimated, for all nonionizing organic compounds except PCDDs and PCDFs, by using the appropriate correlation Equation A-3-4 or A-3-5.

PCDDs and PCDFs For PCDDs and PCDFs, the following correlation equation (Karickhoff, Brown, and Scott 1979) was used to calculate K_{oc} values, as cited by U.S. EPA (1994a).

$$\log K_{oc} = \log K_{ow} - 0.21 \qquad (n = 10, \ r^2 = 1.0) \qquad \text{Equation A-3-7}$$

- Karickhoff, S.W., D.S. Brown, and T.A. Scott. 1979. "Sorption of Hydrophobic Pollutants on Natural Sediments." *Water Resources.* 13:241-248.

Metals For metals, no K_{oc} values were found in the literature. K_{oc} values for metals were not provided in the primary guidance documents, because of the stated assumption that organic carbon in soils does not play a major role in partitioning in soil and sediments. For metals, soil/sediment-water partitioning coefficients (Kd) were obtained directly from experimental measurements (see Kd discussion).

Note: For compounds in which a K_{ow} correlation equation was used to calculate a K_{oc} value, K_{ow} values recommended for each compound in this HHRAP were used.

A3.3.8   Partitioning Coefficients for Soil-Water (Kd_s), Suspended Sediment-Surface Water (Kd_{sw}), and Bottom Sediment-Sediment Pore Water (Kd_{bs})

Partition coefficients (Kd) describe the partitioning of a compound between sorbing material, such as soil, soil pore-water, surface water, suspended solids, and bed sediments. For organic compounds, Kd has been estimated to be a function of the organic-carbon partition coefficient and the fraction of organic carbon in the partitioning media. For metals, Kd is assumed to be independent of the organic carbon in the partitioning media and, therefore, partitioning is similar in all sorbing media.

The soil-water partition coefficient (Kd_s) describes the partitioning of a compound between soil pore-water and soil particles, and strongly influences the release and movement of a compound into the subsurface soils and underlying aquifer. The suspended sediment-surface water partition coefficient (Kd_{sw}) coefficient describes the partitioning of a compound between surface water and suspended solids or sediments. The bed sediment-sediment pore-water partition coefficient (Kd_{bs}) coefficient describes the partitioning of a compound between the bed sediments and bed sediment pore-water.

Organics For organics (including PCDDs and PCDFs), soil organic carbon is assumed to be the dominant sorbing component in soils and sediments. Therefore, Kd values were calculated using the following fraction organic carbon (f_{OC}) correlation equations:

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$$Kd_s = f_{oc,s} \cdot K_{oc} \qquad \text{Equation A-3-8a}$$

$$Kd_{sw} = f_{oc,sw} \cdot K_{oc} \qquad \text{Equation A-3-8b}$$

$$Kd_{bs} = f_{oc,bs} \cdot K_{oc} \qquad \text{Equation A-3-8c}$$

- U.S. EPA. 1993d. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Office of Health and Environmental Assessment. Office of Research and Development. EPA-600-AP-93-003. November 10.

U.S. EPA (1993d), from literature searches, states that f_{OC} could range as follows:

- 0.002 to 0.024 in soils—for which a mid-range value of $f_{oc,s}$ = 0.01 generally can be used.
- 0.05 to 0.1 in suspended sediments—for which a mid-range value of $f_{oc,sw}$ = 0.075 generally can be used.

- 0.03 to 0.05 in bottom sediments—for which a mid-range value of $f_{oc,bs}$ = 0.04 generally can be used.

Consistent with the primary guidance documents, this HHRAP uses mid-range f_{oc} values recommended by U.S. EPA (1993d). *Kd* values were calculated using K_{oc} values recommended for each compound in this HHRAP.

Metals For metals (except mercury), *Kd* is governed by factors other than organic carbon, such as pH, redox, iron content, cation exchange capacity, and ion-chemistry. Therefore, *Kd* values for metals cannot be calculated using the same correlation equations specified for organic compounds. Instead, *Kd* values for the metals must be obtained directly from literature sources. *Kd* values for all metals, except lead, were obtained from U.S. EPA (1996b). U.S. EPA (1996b) provides values for *Kd* that are based on pH, and are estimated by using the MINTEQ2 model, which is a geochemical speciation model. The MINTEQ2 model analyses were conducted under a variety of geochemical conditions and metal concentrations. The MINTEQ2 pH-dependent *Kd* values were estimated by holding constant the iron oxide at a medium value and the f_{oc} at 0.002. For arsenic, hexavalent chromium, selenium, and thallium, empirical pH-dependent *Kd* values were used.

U.S. EPA (1995b) also recommended *Kd* values estimated using the MINTEQ2 model. U.S. EPA (1994f) and NC DEHNR (1997) provided *Kd* values obtained from several literature sources, depending on the compound; however, the *Kd* values are identical in all of the primary guidance documents.

The MINTEQ2 model values in U.S. EPA (1996b) were comparable to the values in the primary guidance documents. In addition, because organic carbon does not play a major role in partitioning for the metals, U.S. EPA (1994f) assumed that the partitioning is the same, regardless of the soil, suspended sediment, or

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bottom sediment phase. Therefore, in this HHRAP, values for partitioning coefficients Kd_s, Kd_{sw}, and Kd_{bs} for the metals are assumed to be the same.

Kd value for lead was obtained from the following:

- Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. "Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides Through Agriculture." Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Mercuric Compounds Kd_s, Kd_{sw}, and Kd_{bs} values for mercury, mercuric chloride, and methyl mercury were obtained from U.S. EPA (1996b). *Kd* values for mercuric chloride and methyl mercury were obtained from U.S. EPA (1997g).

A3.3.9   Soil Loss Constant Due to Degradation (*ksg*)

Soil loss constant due to degradation (*ksg*) reflects loss of a compound from the soil by processes other than leaching. Degradation rates in the soil media include biotic and abiotic mechanisms of transformation. Abiotic degradation includes photolysis, hydrolysis, and redox reactions. Hydrolysis and redox reactions can be significant abiotic mechanisms in soil (U.S. EPA 1990).

The following document states that degradation rates can be assumed to follow first order kinetics in a homogenous media:

- Lyman , W.J., W.F. Reehl, and D.H. Rosenblatt. 1982. *Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds*. McGraw-Hill Book Company. New York, New York.

Therefore, the half-life ($t_{½}$) of compounds can be related to the degradation rate constant (*ksg*) as follows:

$$ksg = \frac{0.693}{t_{½}}$$ Equation A-3-9

Ideally, *ksg* is the sum of all biotic and abiotic rate constants in the soil. Therefore, if the $t_{½}$ for all of the mechanisms of transformation are known, the degradation rate can be calculated using Equation A-3-9. However, literature sources generally do not provide sufficient data for all such mechanisms, especially for soil.

Organics For organics (except PCDDs and PCDFs), *ksg* values were calculated using half-life soil values obtained from the following document:

- Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., and Michalenko, E.M. 1991. *Handbook of Environmental Degradation Rates*. Lewis Publishers. Chelsea, Michigan.

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Half-life values provided in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) indicate the disappearance of a substance in ground water or soil; with the principal degradation mechanisms being biodegradation and hydrolysis. Values reported were highly variable because of the different methods used for measurements, in addition to the various controlling factors that could affect them. Therefore, Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) provided a range of half-life values found in the literature, usually for the fastest reaction mechanism,. *Ksg* values recommended in this HHRAP were calculated with the high-end half-life values.

U.S. EPA (1994b) also cited values obtained from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991). NC DEHNR (1997) cited values that are comparable to *ksg* values calculated by using half-life values obtained from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).

PCDDs and PCDFs For PCDDs and PCDFs, *ksg* values were calculated from half-life values in soil obtained from Mackay, Shiu, and Ma (1992). For 2,3,7,8-TCDD, *ksg* value was obtained from U.S. EPA (1994a); which discussed experimental studies that were conducted on PCDDs and PCDFs degradation mechanisms. U.S. EPA (1994a) summarized the degradation of PCDDs and PCDDs as follows:

- A few experimental studies have shown possible biological degradation of TCDDs. However, the studies conclude that microbial action is very slow for PCDDs under optimum conditions, with the degradation rates probably higher with decreasing chlorination. PCDFs were found to be extremely stable to biological degradation.

- Abiotic degradation, such as photolysis, appears to be the most significant natural degradation mechanism for PCDDs and PCDFs. Experimental studies have shown that PCDDs and PCDFs undergo photolysis in the presence of a suitable hydrogen donor. No information was available to show that other abiotic degradation mechanisms, such as oxidation and hydrolysis, are important under environmentally relevant conditions.

Metals For the metals, NC DEHNR (1997) cites *ksg* values of zero. Literature states that the metals are transformed, but not degraded, by such mechanisms; therefore, *ksg* values are not applicable to metals.

Mercuric Compounds For mercury, mercuric chloride, and methylmercury, U.S. EPA (1997g) recommended *ksg* values of zero.

A3.3.10 Fraction of Pollutant Air Concentration in the Vapor Phase (*F_v*)

Organics For organics, the fraction of pollutant air concentration in the vapor phase (*F_v*) was calculated using the following equation:

$$Fv = 1 - \frac{c\, S_T}{p^{\circ}_{L} + c\, S_T}$$

Equation A-3-10

- Junge, C. E. 1977. *Fate of Pollutants in the Air and Water Environments*, Part I; Suffet, I. H., Ed.; Wiley; New York. Pages 7-26.

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If the compound is a liquid at ambient temperatures (that is, when p°_L is known), Equation A-3-10 calculates F_v using the vapor pressure value recommended for that compound in this HHRAP. If the compound is a solid at ambient temperatures (that is, when p°_S is known), the following equation (Bidleman 1988) was used to calculate p°_L from p°_S, for use in Equation A-3-10:

$$\ln \left(\frac{p^{\circ}_L}{p^{\circ}_S}\right) = \frac{\Delta S_f}{R} \frac{(T_m - T)}{T} \qquad\qquad \text{Equation A-3-11}$$

where

c	=	Junge constant = 1.7×10^{-04} (atm-cm)
p°_L	=	Liquid phase vapor pressure of compound (atm)
p°_s	=	Solid phase vapor pressure of compound (atm)
R	=	Universal ideal gas constant (atm-m^3/mole-K)
ΔS_f	=	Entropy of fusion [$\Delta S_f/R$ = 6.79 (unitless)]
S_T	=	Whitby's average surface area of particulates (aerosols)
T_a	=	Ambient air temperature (K)—assumed to be 25°C or 298 K

This equation was adopted from:

- Bidleman, T.F. 1988. "Atmospheric Processes." *Environmental Science and Technology.* Volume 22. Number 4. Pages 361-367.

According to Bidleman (1988), Equation A-3-10 assumes that the Junge constant (*c*) is constant for all compounds. However, *c* can depend on (1) the compound (sorbate) molecular weight, (2) the surface concentration for monolayer coverage, and (3) the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate.

The primary guidance documents used Equations A-3-10 and A-3-11 to compute *Fv*. However, it is not clear what values of *S*, *T*, and *Vp* values were used to calculate values for F_v. For example, U.S. EPA (1994f) calculated F_v values at (*T*) of 11°C. Because of inconsistencies in the values in the primary guidance documents, *Fv* values in the primary guidance documents were not recommended for use in this HHRAP. F_v values were calculated using the recommended values of *Vp* and T_m provided in this HHRAP for each compound.

Metals Consistent with U.S. EPA (1994f), all metals (except mercury) are assumed to be present in the particulate phase and not in the vapor phase (*Vp* = 0), and assigned F_v values of zero.

Mercuric Compounds Mercury and mercuric chloride are relatively volatile and exist in the vapor phase (U.S. EPA 1997g). Therefore, the *Fv* value recommended in this HHRAP for mercury was calculated using Equations A-3-10 and A-3-11.

Based on discussions on mercury presented in Chapter 2 of this HHRAP, *Fv* values of 1.0 for mercury (same as calculated using Equations A-3-10 and A-3-11), and 0.85 for mercuric chloride were estimated.

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Consistent with information provided in U.S. EPA (1997g), methyl mercury is assumed not to exist in the air phase and, therefore, assigned an Fv of zero.

A3.4   BIOCONCENTRATION AND BIOTRANSFER FACTORS FOR PLANTS

A3.4.1   Root Concentration Factor (RCF)

The root concentration factor (RCF) is used to calculate the belowground transfer of compound from soil to a root vegetable.

Organics For organics, the following correlation equation was used to calculate RCF :

$$\log (RCF - 0.82) = 0.77 \log K_{ow} - 1.52 \qquad \text{Equation A-3-12}$$

This equation was obtained from the following document:

- Briggs, G.G., R.H. Bromilow, and A.A. Evans, 1982. "Relationships Between Lipophilicity and Root Uptake and Translocation of Non-ionized Chemicals by Barley." *Pesticide Science.* Volume 13. Pages 495-504.

This equation estimates a RCF value in fresh weight (FW) units, which was then converted to dry weight (DW) units using a moisture content of 87 percent in root vegetables (U.S. EPA 1997h; Pennington 1994). K_{ow} values recommended in this HHRAP were used to calculate each RCF value.

The primary guidance documents also recommended using correlation Equation A-3-12. U.S. EPA (1994a) adopted this correlation equation for calculating exposure to dioxin-like compounds.

Metals For metals, no referenced RCF values were available in published literature. However, plant-soil biotransfer factors for root vegetables ($Br_{rootveg}$) were available in the literature and, therefore, RCF values, which were used to calculate $Br_{rootveg}$ values, are not required for the metals.

Mercuric Compounds No RCF values were available for mercury, mercuric chloride, and methyl mercury in the literature. However, plant-soil biotransfer factors for root vegetables ($Br_{rootveg}$) were available in U.S. EPA (1997g) and, therefore, RCF values, which were used to calculate $Br_{rootveg}$ values, are not required for the mercuric compounds.

A3.4.2   Plant-Soil Bioconcentration Factors in Root Vegetables ($Br_{rootveg}$)

The plant-soil bioconcentration factor for compounds in root vegetables ($Br_{rootveg}$) accounts for uptake from soil to the belowground root vegetables or produce. Discussion on $Br_{rootveg}$ values also is provided in Section A3.4.3.

Organics For organics, the following equation, obtained from U.S. EPA (1995b), was used to calculate values for $Br_{rootveg}$ on a dry weight basis:

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$$Br_{rootveg} = \frac{RCF}{Kd_s}$$ Equation A-3-13

$Br_{rootveg}$ values were calculated by dividing the RCF value with the Kd_s values provided in this HHRAP.

Metals $Br_{rootveg}$ values for metals (except nickel, cadmium, selenium, and arsenic) were obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values in Baes, Sharp, Sjoreen, and Shor (1984) are dry weight values provided for nonvegetative (reproductive) growth, such as tubers.

For nickel, cadmium, selenium, and arsenic, $Br_{rootveg}$ values were obtained from the following document:

- U.S. EPA. 1992b. *Technical Support Document for the Land Application of Sewage Sludge. Volumes I and II*. EPA 822/R-93-001a. Office of Water. Washington, D.C.

For nickel, cadmium, selenium, and arsenic—$Br_{rootveg}$ values were calculated by multiplying the uptake slope factors [(μg COPC/g DW plant)/(kg COPC applied/hectare)] for root vegetables by a conversion factor of 2×10^9 g/hectare soil. In deriving the conversion factor, U.S. EPA (1992b) assumed a soil average dry bulk density of 1.33 g/cm³ and a soil incorporation depth of 15 cm.

Mercuric Componds $Br_{rootveg}$ values for mercuric chloride and methyl mercury were obtained from U.S. EPA (1997g) on a dry weight basis. Elemental mercury is assumed not to deposit onto soils; and therefore, it is assumed that there is no plant uptake through the soil. Therefore, a $Br_{rootveg}$ value for elemental mercury is not applicable for this HHRAP.

A3.4.3   Plant-Soil Bioconcentration Factors for Aboveground Produce (Br_{ag}) and Forage (Br_{forage})

The plant-soil bioconcentration factor (Br) for aboveground produce accounts for the uptake from soil and the subsequent transport of COPCs through the roots to the aboveground plant parts. As addressed in U.S. EPA (1995b), the Br value for organics is a function of water solubility, which is inversely proportional to K_{ow}. The Br value for metals is a function of the bioavailability of the compounds in soil.

Primarily, two parameters—Br_{ag} and Br_{forage}—are presented in this Appendix. For all organics including PCDDs and PCDFs, (1) the subscript "*ag*" represents aboveground produce which applies to exposed fruits and vegetables, and protected fruits and vegetables, and (2) the subscript "*forage*" represents forage, but the values also apply to silage and grain. For metals, (1) aboveground fruits (both exposed and protected) are represented by $Br_{ag\,(fruit)}$; (2) aboveground vegetables (both exposed and protected) are represented by $Br_{ag(veg)}$, (3) forage is represented by Br_{forage}, but the values also apply to silage, and (4) grains are represented by Br_{grain}.

The U.S. EPA (1995b) and NC DEHNR (1997) guidance documents provided` two parameters—$Br_{leafy\,veg}$ and Br_{forage}. The subscript "leafy veg" represents leafy vegetables and "forage" represents forage, silage, and grain. U.S. EPA (1994f) provides only one Br value for each COPC and does not provide a distinction between leafy vegetables or aboveground produce, forage, and root vegetables.

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Organics For organics, the following correlation equations were used to calculate values for Br_{ag} and Br_{forage} on a dry weight basis:

$$\log Br_{ag} = 1.588 - 0.578\ (\log K_{ow}) \qquad (n = 29,\ r = 0.73) \qquad \text{Equation A-3-14a}$$

$$\log Br_{forage} = 1.588 - 0.578\ (\log K_{ow}) \qquad (n = 29,\ r = 0.73) \qquad \text{Equation A-3-14b}$$

These correlation equations were obtained from;

- Travis, C.C. and A.D. Arms. 1988. Bioconcentration of Organics in Beef, Milk, and Vegetation. *Environmental Science and Technology.* 22:271-274.

Travis and Arms (1988) developed a correlation equation for vegetation and does not distinguish between aboveground produce and forage or silage or grain. Due to lack of literature data, the Travis and Arms (1988) correlation equation was used to calculate Br values for both aboveground produce and forage. The K_{ow} value recommended for each organic compound in this HHRAP was used.

This approach is consistent with that used in the primary guidance documents. However, it should be noted that the Travis and Arms (1988) correlation equations were derived from experiments conducted on compound classes such as DDT, pesticides, PCDDs, PCDFs, and PCBs. Therefore, further research is needed to evaluate the applicability and limitations associated with the use of such correlation equations to all classes of compounds.

Metals For metals—nickel, cadmium, selenium, zinc, and arsenic—Br values were derived from uptake slope factors provided in the following document:

- U.S. EPA. 1992b. *Technical Support Document for the Land Application of Sewage Sludge.* Volumes I and II. EPA 822/R-93-001a. Office of Water. Washington, DC.

Uptake slopes provided in U.S. EPA (1992b) are the ratio of COPC concentration in dry weight plant tissue to the mass of COPC applied per hectare soil. These uptake slopes were multiplied by 2×10^9 g/hectare soil to convert to Br values. The conversion factor was derived using the U.S. EPA (1992b) assumed soil bulk density of 1.33 g/cm^3, and incorporation depth of 15 cm.

For the remaining metals (excluding mercury), Br values were obtained from Baes, Sharp, Sjoreen, and Shor (1984). Baes, Sharp, Sjoreen, and Shor (1984) described biotransfer factors (on a dry weight basis) from plant-soil uptake for (1) vegetative growth (leaves and stems) "Bv"; and (2) nonvegetative or reproductive growth (fruits, seeds, and tubers) "Br". Note that Bv is defined in this HHRAP as the air-to-plant biotransfer factor.

This HHRAP uses the following methodology to derive Br values on a dry weight basis:

a.   For nickel, cadmium, selenium, zinc, and arsenic, $Br_{ag\ (fruit)}$ values were calculated by multiplying the uptake slope factors with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S.

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EPA (1992b) for garden fruits. For all other metals, "Br" values for nonvegetative growth (reproductive) provided in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{ag\,(fruit)}$ values.

b. For nickel, cadmium, selenium, zinc, and arsenic, $Br_{ag\,(veg)}$ values were calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2×10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1992b). For all other metals, "Br" values for nonvegetative (reproductive) growth and "Bv" values for vegetative growth—obtained from Baes, Sharp, Sjoreen, and Shor (1984)—were weighted as 75% (reproductive) and 25% vegetative. The resulting values were adopted as $Br_{ag\,(veg)}$ values.

c. For nickel, cadmium, selenium, zinc, and arsenic, Br_{forage} values were calculated by multiplying the uptake slope factors with a conversion factor of 2×10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables. Br_{forage} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984). "Bv" values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{forage}.

d. For nickel, cadmium, selenium, zinc, and arsenic, Br_{grain} values were calculated by multiplying the uptake slope factors with a conversion factor of 2×10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals. Br_{grain} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). "Br" values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{grain}.

The primary guidance documents used the following methodology to obtain Br values for metals:

1. U.S. EPA (1994f) provided only one Br value and did not distinguish between leafy vegetables or aboveground produce, forage, and root vegetables.

2. U.S. EPA (1995b) used:

    a. "Bv" values in Baes, Sharp, Sjoreen, and Shor (1984), provided for vegetative growth, were used for $Br_{leafy\,veg}$ values for antimony, barium, beryllium, copper, chromium, lead, molybdenum, silver, thallium, and vanadium.

    b. "Bv" values in Baes, Sharp, Sjoreen, and Shor (1984), provided for vegetative growth, were used for Br_{forage} values for antimony, barium, beryllium, chromium, lead, silver, thallium, and vanadium.

    c. "Br" values in Baes, Sharp, Sjoreen, and Shor (1984), provided for nonvegetative growth, were used for $Br_{root\,veg}$ values for antimony, barium, beryllium, copper, chromium, lead, molybdenum, silver, thallium, and vanadium.

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All other values were obtained from plant uptake response slope factors calculated from field data (e.g., metal loading rates and soil metal concentrations) contained in various literature sources.

3. NC DEHNR (1997):

   a. Uses "Bv" values in Baes, Sharp, Sjoreen, and Shor (1984), provided for vegetative growth, for $Br_{leafy\,veg}$ and Br_{forage} values. NC DEHNR (1997) does not differentiate between forage and leafy vegetables (aboveground produce).

   b. $Br_{rootveg}$ values were not available.

**Mercuric Compounds** Br_{ag} and Br_{forage} values on a dry weight basis for mercuric chloride and methyl mercury were obtained from U.S. EPA (1997g). Elemental mercury is assumed not to deposit onto soils. Therefore, it is assumed that there is no plant uptake through the soil. This is based on the assumptions made regarding speciation and fate and transport of mercury from stack emissions (see Chapter 2).

If field data suggests otherwise, the same methodology that was used to derive Br values from Baes, Sharp, Sjoreen, and Shor (1984) data could be used for elemental mercury. However, for purposes of this HHRAP, it should be noted that uptake of mercury from air into the aboveground plant tissue is assumed to primarily consist of the divalent form of mercury. Therefore, a Br value for the aboveground plant parts for elemental mercury is not applicable for this HHRAP.

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A3.4.4   Air-to-Plant Biotransfer Factors for Aboveground Produce (Bv_{ag}) and Forage (Bv_{forage})

The air-to-plant biotransfer factor (Bv) is defined as the ratio of COPC concentration in aboveground plant parts to the COPC concentration in air. Bv values for all organics and metals, were calculated only for aboveground exposed produce (both fruits and vegetables). For this HHRAP, aboveground protected produce (both fruits and vegetables) and belowground produce were assumed to be protected from air-to-plant transfer. According to U.S. EPA (1995b), root vegetables are assumed to be also protected from air-to-plant transfer.

Organics For organics (excluding PCDDs and PCDFs), the air-to-plant biotransfer factor for aboveground produce (Bv_{ag}) and forage (Bv_{forage}) were calculated using correlation equations derived for azalea leaves in the following documents:

- Bacci E., D. Calamari, C. Gaggi, and M. Vighi. 1990. "Bioconcentration of Organic Chemical Vapors in Plant Leaves: Experimental Measurements and Correlation." *Environmental Science and Technology.* Volume 24. Number 6. Pages 885-889.

- Bacci E., M. Cerejeira, C. Gaggi, G. Chemello, D. Calamari, and M. Vighi. 1992. "Chlorinated Dioxins: Volatilization from Soils and Bioconcentration in Plant Leaves." *Bulletin of Environmental Contamination and Toxicology.* Volume 48. Pages 401-408.

Bacci, Cerejeira, Gaggi, Chemelo, Calamari, and Vighi (1992) developed a correlation equation by using data collected for the uptake of 1,2,3,4-tetrachlorodibenzo-p-dioxin (TCDD) in azalea leaves, and data obtained from Bacci, Calamari, Gaggi, and Vighi (1990). The Bv obtained was then evaluated for 14 organic compounds to develop a correlation equation with K_{ow} and H. Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) derived the following equations without distinguishing between forage and aboveground produce:

$$\log B_{vol} = 1.065 \log K_{ow} - \log \left(\frac{H}{RT}\right) - 1.654 \qquad (r = 0.957) \qquad \text{Equation A-3-15a}$$

where

$$Bv = \frac{\rho_{air} \cdot B_{vol}}{(1 - f_{water}) \cdot \rho_{forage}} \qquad \qquad \text{Equation A-3-15b}$$

B_{vol}	=	Volumetric air-to-plant biotransfer factor (fresh-weight basis)
Bv	=	Mass-based air-to-plant biotransfer factor (dry-weight basis)
ρ_{air}	=	1.19 g/L (Weast 1981)
ρ_{forage}	=	770 g/L (Macrady and Maggard 1993)
f_{water}	=	0.85 (fraction of forage that is water—Macrady and Maggard [1993])

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Equations A-3-13 and A-3-14 were used to calculate Bv values using the recommended values of H and K_{ow} provided in this HHRAP for a T of 25 °C or 298.1 K. The resulting Bv values were adopted for both forage (Bv_{forage}) and aboveground produce (Bv_{ag}). The primary guidance documents also used Equations A-3-13 and A-3-14 to calculate Bv values. The following uncertainty should be noted when using these variables:

- For organics (except PCDDs and PCDFs), U.S. EPA (1993d) recommended that Bv values be reduced by a factor of 10 before use. This was based on the work conducted by U.S. EPA (1993d) for U.S. EPA (1994a) as an interim correction factor. Welsch-Pausch, McLachlan, and Umlauf (1995) conducted experiments to determine concentrations of PCDDs and PCDFs in air and resulting biotransfer to welsh ray grass. This was documented in the following:

  - Welsch-Pausch, K.M. McLachlan, and G. Umlauf. 1995. "Determination of the Principal Pathways of Polychlorinated Dibenzo-p-dioxins and Dibenzofurans to Lolium Multiflorum (Welsh Ray Grass)". *Environmental Science and Technology.* 29: 1090-1098.

  A follow-up study based on Welsch-Pausch, McLachlan, and Umlauf (1995) experiments was conducted by Lorber (1995) (see discussion below for PCDDs and PCDFs). In a following publication, Lorber (1997) concluded that the Bacci factor reduced by a factor of 100 was close in line with observations made by him through various studies, including the Welsch-Pausch, McLachlan, and Umlauf (1995) experiments. Therefore, for this HHRAP, Bv values were calculated using the Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) correlation equations and then reduced by a factor of 100 for all organics, excluding PCDDs and PCDFs.

PCDDs and PCDFs For PCDDs and PCDFs, Bv values, on a dry weight basis, were obtained from the following:

- Lorber, M. 1995. "Development of an Air-to-plant Vapor Phase Transfer for Dioxins and Furans. Presented at the 15th International Symposium on Chlorinated Dioxins and Related Compounds". August 21-25, 1995 in Edmonton, Canada. Abstract in *Organohalogen Compounds.* 24: 179-186.

U.S. EPA (1993d) stated that, for dioxin-like compounds, the use of the Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) equations may overpredict Bv values by a factor of 40. This was because the Bacci, Calamari, Gaggi, and Vighi (1990) and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) experiments did not take photodegradation effects into account. Therefore, Bv values calculated using Equations A-3-13 and A-3-14 were recommended to be reduced by a factor of 40 for dioxin-like compounds. This procedure was also followed by the primary guidance documents.

However, according to Lorber (1995), the Bacci algorithm divided by 40 may not be appropriate because (1) the physical and chemical properties of dioxin congeners are generally outside the range of the 14 organic compounds used by Bacci, Calamari, Gaggi, and Vighi (1990), and (2) the factor of 40 derived from one experiment on 2,3,7,8-TCDD may not apply to all dioxin congeners.

Welsch-Pausch, McLachlan, and Umlauf (1995) conducted experiments to obtain data on uptake of

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PCDDs and PCDFs from air to *Lolium Multiflorum* (Welsh Ray grass). The data includes grass concentrations and air concentrations for dioxin-congener groups, but not the invidual congeners. Lorber (1995) used data from Welsch-Pausch, McLachlan, and Umlauf (1995) to develop an air-to-leaf transfer factor for each dioxin-congener group. *Bv* values developed by Lorber (1995) were about an order of magnitude less than values that would have been calculated using the Bacci, Calamari, Gaggi, and Vighi (1990) and 1992) correlation equations. Lorber (1995) speculated that this difference could be attributed to several factors including experimetal design, climate, and lipid content of plant species used.

Br values recommended for PCDDs and PCDFs in this HHRAP were obtained from the experimentally derived values of Lorber (1995). However, Lorber (1995) stated that these values should be considered carefully by users of this methodology because of the inherent uncertainties associated with the data.

Metals For metals, no literature sources were found for the *Bv* values. U.S. EPA (1995b) quoted from the following document, that metals were assumed not to experience air to leaf transfer:

- Belcher, G.D., and C.C. Travis. 1989. "Modeling Support for the RURA and Municipal Waste Combustion Projects: Final Report on Sensitivity and Uncertainty Analysis for the Terrestrial Food Chain Model." Interagency Agreement No. 1824-A020-A1. Office of Risk Analysis, Health and Safety Research Division. Oak Ridge National Laboratory. Oak Ridge, Tennessee. October.

Consistent with the above references, *Bv* values for metals (excluding elemental mercury) were assumed to be zero for this HHRAP.

Mercuric Compounds Mercury emissions are assumed to consist of both the elemental and divalent forms. However, only small amounts of elemental mercury is assumed to be deposited (see Chapter 2). Elemental mercury either dissipates into the global cycle or is converted to the divalent form. Methyl mercury is assumed not to exist in the stack emissions or in the air phase. Consistent with various discussions in Chapter 2 concerning mercury, (1) elemental mercury reaching or depositing onto the plant surfaces is negligible, and (2) biotransfer of methyl mercury from air is zero. This is based on assumptions made regarding speciation and fate and transport of mercury from stack emissions. Therefore, the *Bv* value for (1) elemental mercury was assumed to be zero, and (2) methyl mercury was assumed not to be applicable. *Bv* values for mercuric chloride (dry weight basis) were obtained from U.S. EPA (1997g).

If field data suggests otherwise, *Bv* values (1) provided in U.S. EPA (1997g) for methyl mercury can be used and (2) need to be determined for elemental mercury. It should be noted that uptake of mercury from air into the aboveground plant tissue is primarily in the divalent form. A part of the divalent form of mercury is assumed to be converted to the methyl mercury form once in the plant tissue.

A3.5   BIOTRANSFER FACTORS FOR ANIMALS

The biotransfer factor for animals (*Ba*) is the ratio of COPC concentration in fresh weight animal tissue to the daily intake of COPC by the animal.

A3.5.1   Biotransfer Factors for Beef (Ba_{beef}) and Milk (Ba_{milk})

Organics For organics (except PCDDs and PCDFs), the following correlation equations were used to calculate biotransfer factors for beef (Ba_{beef}) and milk (Ba_{milk}) on a fresh weight basis:

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$$\log Ba_{beef} = -7.6 + \log K_{ow} \quad (n = 36, \, r = 0.81) \qquad \text{Equation A-3-16}$$

$$\log Ba_{milk} = -8.1 + \log K_{ow} \quad (n = 28, \, r = 0.74) \qquad \text{Equation A-3-17}$$

These equations were obtained from Travis and Arms (1988). The primary guidance documents also recommend the use of the correlation equations from Travis and Arms (1988).

The K_{ow} values recommended in this HHRAP were used in correlation Equations A-3-15 and A-3-16 to calculate Ba_{beef} and Ba_{milk} values for all organic compounds except PCDDs and PCDFs.

The Travis and Arms (1988) correlation equations were derived from experiments conducted on compound classes such as DDT, pesticides, PCDDs, PCDFs, and PCBs. As further literature is developed for other classes of compounds, the Travis and Arms (1988) correlation equations should be evaluated concerning their applicability to all classes of organic compounds.

PCDDs and PCDFs Ba_{beef} and Ba_{milk} values on a fresh weight basis for PCDDs and PCDFs were obtained from:

- U.S. EPA. 1995a. *Further Studies for Modeling the Indirect Exposure Impacts from Combustor Emissions.* Memorandum from Mathew Lorber, Exposure Assessment Group, and Glenn Rice, Indirect Exposure Team, Environmental Criteria and Assessment Office. Washington, DC. January 20.

The Travis and Arms (1988) correlation equations were derived from experiments conducted on compound classes which included PCDDs and PCDFs. Therefore, it may appear appropriate to use correlation Equations A-3-15 and A-3-16 to calculate Ba_{beef} and Ba_{milk} values for PCDDs and PCDFs. However, literature sources have reported that it is not appropriate to use the Travis and Arms (1988) correlation equations to calculate beef and milk biotransfer factors for dioxin-like compounds. U.S. EPA (1995a) discussed the inappropriateness of using the Travis and Arms (1988) correlation equations for dioxin-like compounds:

- The Travis and Arms (1988) correlation equations overestimate Ba_{beef} and Ba_{milk} values for dioxin-like compounds, based on the following experimental studies conducted on lactating cows:

    - McLachlan, M.S., H. Thoma, M. Reissinger, and O. Hutzinger. 1990. "PCDD/F in an Agricultural Food Chain. Part I: PCDD/F Mass Balance of a Lactating Cow." *Chemosphere.* Volume 20 (Numbers 7-9). Pages 1013-1020.

- Ba values would increase with increasing K_{ow} using the Travis and Arms (1988) correlation equations; whereas, U.S. EPA (1994a) stated that Ba values for compounds with a log K_{ow} from 6.5 to 8.0 (such as the dioxin-like compounds) would actually decrease with increasing K_{ow}. This could be a result of greater rates of metabolism for

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organic compounds of higher K_{ow}, or only for the dioxins, leading to lower concentrations in the animal food products.

- Ba_{beef} and Ba_{milk} values generated from the McLachlan, Thoma, Reissinger, and Hutzinger (1990) experiments were recommended instead of the Travis and Arms (1988) estimated values. U.S. EPA (1995a) derived Ba values using the McLachlan, Thoma, Reissinger, and Hutzinger (1990) experimentally derived data. U.S. EPA (1995a) assumed that milk is 3.5 percent fat and that beef is 19 percent fat. Therefore, Ba_{beef} values would be 5.43 times (19/3.5) higher than for milk with these fat content assumptions.

Values recommended in this HHRAP also assumed that milk is 3.5 percent fat and that beef is 19 percent fat. Consistent with U.S. EPA (1995a), biotransfer factors for beef would be 5.43 times (25/3.68) higher than for milk. Therefore, in this HHRAP, Ba_{milk} values for PCDDs and PCDFs were obtained from U.S. EPA (1995a), and Ba_{beef} values were calculated by increasing Ba_{milk} values by a factor of 5.43.

U.S. EPA (1994f) cited Ba_{beef} and Ba_{milk} values obtained through personal communication with Matthew Lorber, Exposure Assessment Group, Office of Research and Development. These were interim values intended to represent dioxin TEQs by weighting data for all dioxin and furan congeners with nonzero toxicity equivalent factors (TEF). U.S. EPA (1995b) stated that the lipophilic nature of PCDDs, PCDFs, and PCBs causes them to transfer directly to the lipid within the beef and milk rather than adsorb to both beef muscle and beef fat or, in the case of milk, milk and milk fat. U.S. EPA (1995b) stated that an alternative methodology was used to calculate PCB, PCDD, and PCDF concentrations in beef and milk. Therefore, the beef and milk biotransfer factors concept was not applicable to PCBs, PCDDs, and PCDFs.

Metals For metals (except cadmium, mercury, selenium, and zinc), Ba_{beef} and Ba_{milk} values on a fresh weight basis were obtained from Baes, Sharp, Sjoreen, and Shor (1984). For cadmium, selenium, and zinc, U.S. EPA (1995a) cited Ba values derived by dividing uptake slopes [(g COPC/kg DW tissue)/(g COPC/kg DW feed)], obtained from U.S. EPA (1992b), by a daily consumption rate of 20 kg DW per day for beef and dairy cattle.

All primary guidance documents also obtain Ba values from these sources. Therefore, values presented in this HHRAP are obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals except cadmium, selenium, and zinc. For cadmium, selenium, and zinc, Ba values were calculated using uptake slope factors and consumption rates provided in U.S. EPA (1992b) and U.S. EPA (1995a), and converting the result to a fresh weight basis by assuming a moisture content of 87 percent in milk and 70 percent in beef. Moisture content in beef and milk were obtained from the following:

- U.S. EPA. 1997h. *Exposure Factors Handbook.* "Food Ingestion Factors". Volume II. EPA/600/P-95/002Fb. August.

- Pennington, J.A.T. 1994. *Food Value of Portions Commonly Used.* Sixteenth Edition. J.B. Lippincott Company, Philadelphia.

The calculated fresh weight Ba_{beef} and Ba_{milk} values are recommended for use in this HHRAP.

Mercuric Compounds Elemental mercury is assumed to neither deposit onto soils or transfer to the aboveground plant parts. Therefore, there is no transfer of elemental mercury into animal tissue. Therefore, Ba values for elemental mercury are reported in this HHRAP as not applicable. This based on

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assumptions made regarding speciation and fate and transport of mercury from stack emissions (see Chapter 2).

If field data suggests otherwise, Ba_{beef} and Ba_{milk} values for elemental mercury can be derived from the uptake slope factors provided in U.S. EPA (1992b) and U.S. EPA (1995a); using the same consumption rates discussed earlier for metals like cadmium, selenium, and zinc.

Ba_{beef} and Ba_{milk} values reported in this HHRAP for mercuric chloride and methyl mercury were derived from data in U.S. EPA (1997g). U.S. EPA (1997g) provided Ba_{beef} and Ba_{milk} values for mercury, but did not specify for which form of mercury. Consistent with U.S. EPA 1997g, mercury is assumed to be speciate into 87 percent divalent mercury and 13 percent methyl mercury in herbivore animal tissue. Also, assuming that the Ba_{beef} and Ba_{milk} values provided in U.S. EPA (1997g) were for total mercury in animal tissue, then biotransfer factors in U.S. EPA (1997g) can be apportioned in the fractions assumed to be found in animal tissue. Therefore, values reported in this HHRAP are based on the following:

- Default Ba_{milk} value of 0.02 day/kg DW for mercury obtained from U.S. EPA (1997g) was converted to a fresh weight basis assuming a 87 percent moisture content in milk (U.S. EPA 1997h; and Pennington 1994). The calculated Ba_{milk} (fresh weight) value was multiplied by (1) 0.13 to obtain a value for methyl mercury, and (2) 0.87 to obtain a value for mercuric chloride (divalent mercury).

- Default Ba_{beef} value of 0.02 day/kg DW for mercury obtained from U.S. EPA (1997g) was converted to a fresh weight basis assuming a 70 percent moisture content in beef (U.S. EPA 1997h; and Pennington 1994). The calculated Ba_{beef} (fresh weight) value was multiplied by (1) 0.13 to obtain a value for methyl mercury, and (2) 0.87 to obtain a value for mercuric chloride (divalent mercury).

A3.5.2 Biotransfer Factors for Pork (Ba_{pork})

Organics For organics (except PCDDs and PCDFs), Ba_{pork} values reported in this HHRAP were derived from Ba_{beef} values, assuming that pork is 23 percent fat and beef is 19 percent fat. Therefore, Ba_{pork} values were calculated by multiplying Ba_{beef} values by their fat content ratio of 1.2 (23/19). This calculation is limited by the assumptions that (1) COPCs bioconcentrate in the fat tissues, and (2) there is minimal effect from differences in metabolism and feeding characteristics between beef cattle and pigs.

PCDDs and PCDFs For PCDDs and PCDFs, Ba_{pork} values reported in this HHRAP were calculated using the same methodology used to obtain Ba_{beef} values by U.S. EPA (1995a). Assuming that milk is 3.5 percent fat and that pork is 23 percent fat, biotransfer factors for pork would be 6.57 times (23/3.5) higher than for milk. Therefore, Ba_{pork} values were calculated by increasing Ba_{milk} values by a factor of 6.57. This has the same effect as if the Ba_{pork} values were calculated by multiplying the Ba_{beef} values with the fat content ratio of 1.2 (23/19) between pork and beef, as was adopted for the remaining organic compounds.

Metals For metals (except cadmium, selenium, and zinc), no data was available in the literature to calculate Ba_{pork} values.

For cadmium, selenium, and zinc, U.S. EPA (1995b) reported Ba values derived by dividing uptake slopes [(g COPC/kg DW tissue)/(g COPC/kg DW feed)], obtained from U.S. EPA (1992b), by a daily

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consumption rate of 4.7 kg DW per day for pigs provided in U.S. EPA (1995a). The dry weight Ba_{pork} values (for cadmium, selenium, and zinc) were converted to a fresh weight basis assuming a moisture content of 70 percent in pork (U.S. EPA 1997h; and Pennington 1994). The calculated fresh weight Ba_{pork} values are recommended for use in this HHRAP.

Mercuric Compounds Elemental mercury is assumed not to deposit onto soils or be transferred to the aboveground plant parts.; therefore, there is no transfer of elemental mercury into the animal tissue. Therefore, *Ba* values for elemental mercury are reported in this HHRAP as not applicable. This is based on the assumptions made regarding speciation and fate and transport of mercury from stack emissions (see Chapter 2).

If field data suggests otherwise, Ba_{pork} values for elemental mercury can be derived from the uptake slope factors as provided in U.S. EPA (1992b) and U.S. EPA (1995a), using the same consumption rates discussed earlier for metals like cadmium, selenium, and zinc.

Ba_{pork} values reported in this HHRAP for mercuric chloride and methyl mercury were derived from data in U.S. EPA (1997g). U.S. EPA (1997g) provided Ba_{pork} values for mercury, but did not specify for which form of mercury. Consistent with U.S. EPA (1997g), mercury is assumed to be speciate into 87 percent divalent mercury and 13 percent methyl mercury in herbivore animal tissue. Also, assuming that the Ba_{pork} values provided in U.S. EPA (1997g) were for total mercury in animal tissue, then biotransfer factors in U.S. EPA (1997g) can be apportioned in the fractions it is assumed to be found in animal tissue.

Therefore, the default Ba_{pork} value reported in this HHRAP of 0.00013 day/kg DW for mercury was obtained from U.S. EPA (1997g) and converted to a fresh weight basis assuming a 70 percent moisture content in pork (U.S. EPA 1997h; and Pennington 1994). The calculated Ba_{pork} (fresh weight) value was multiplied by (1) 0.13 to obtain a value for methyl mercury, and (2) 0.87 to obtain a value for mercuric chloride (divalent mercury).

A3.5.3   Biotransfer Factors for Chicken ($Ba_{chicken}$) and Poultry Eggs (Ba_{egg})

Biotransfer factors for chicken ($Ba_{chicken}$) and poultry eggs (Ba_{egg}) are expressed as the ratio of the COPC concentration in the fresh weight tissue to the COPC intake from the feed. Biotransfer factors are calculated from bioconcentration factors for chicken and poultry eggs. BCFs are expressed as the ratio of the COPC concentration in the fresh weight tissue to the COPC concentration in dry weight soil.

The primary guidance documents, except for NC DEHNR (1997) do not evaluate exposure through chicken and eggs. NC DEHNR (1997) considers the chicken and egg ingestion pathways only for exposures to PCDDs and PCDFs.

Organics For organics (except PCDDs and PCDFs), $Ba_{chicken}$ values were derived from Ba_{beef} values by assuming that chicken is 15 percent fat and beef is 19 percent fat. Therefore, $Ba_{chicken}$ values were calculated by multiplying Ba_{beef} values by their fat content ratio of 0.8 (15/19). This calculation is limited by the assumptions that (1) COPCs bioconcentrate in the fat tissues, and (2) there is minimal effect from differences in metabolism or feeding characteristics between beef cattle and chickens. Due to the lack of literature data available on $Ba_{chicken}$ values, this methodology has also been followed by various other risk assessment guidance documents.

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Ba_{eggs} values were calculated using a correlation equation derived and recommended for use in the following:

- California Environmental Protection Agency (CEPA). 1993. "Parameter Values and Ranges for CALTOX." Draft. Office of Scientific Affairs. California Department of Toxic Substances Control. Sacramento, CA. July.

CEPA (1993) derived the following correlation equation obtained from experimental studies conducted on PCDDs and PCDFs using fat-soil and fat-diet partitioning factors in chicken and eggs:

$$\log Ba_{egg} = -5.1 + \log K_{ow} \qquad (n = 64, \ r^2 = 0.61) \qquad \text{Equation A-3-18}$$

The K_{ow} values recommended in this HHRAP were used in correlation Equation A-3-18 to calculate Ba_{egg} values for all organic compounds (except PCDDs and PCDFs).

PCDDs and PCDFs $Ba_{chicken}$ and Ba_{eggs} values were obtained by multiplying the BCF values for chicken and eggs for PCDDs and PCDFs (provided in Table 3 of the following) by the daily consumption rate of soil by chicken:

- Stephens, R.D., M. Petreas, and G.H. Hayward. 1995. "Biotransfer and Bioaccumulation of Dioxins and Furans from Soil: Chickens as a Model for Foraging Animals." *The Science of the Total Environment.* 175: 253-273. July 20.

Stephens, Petreas, and Hayward (1995) conducted experiments to determine the bioavailability and the rate of PCDDs and PCDFs uptake from soil by the foraging chickens. Three groups of White Leghorn chickens were studied—control group, low exposure group, and high exposure group. Eggs, tissues (liver, adipose, and thigh), feed, and feces were analyzed. The Stephens, Petreas, and Hayward (1995) experimental information was intended to explain the relationship between soil PCDDs/PCDFs and human foods and, consequently, provide a basis for setting regulatory limits on allowable concentrations in soil used in agriculture. For this HHRAP, to be conservative, BCF values for chicken thigh meat from the high exposure group were adopted.

Consumption rate of soil by chicken (0.02 kg DW/day) was calculated using the following methodology:

(1) Consumption rate of feed by chicken was obtained from U.S. EPA (1995a), which cites a value of 0.2 kg DW feed/day obtained from various literature sources.
(2) The fraction of feed that is soil (0.1) was obtained from Stephens, Petreas, and Hayward (1995).
(3) Feed consumption rate of 0.2 kg/day was multiplied by the fraction of feed that is soil (0.1), to obtain the soil consumption rate by chicken of 0.2 x 0.1 = 0.02 kg DW soil/day.

Therefore, the BCF values for chicken and eggs were multiplied by a chicken consumption rate of soil of 0.02 kg(DW)/day, respectively, to obtain $Ba_{chicken}$ and Ba_{egg} values reported in this HHRAP.

Metals $Ba_{chicken}$ and Ba_{egg} values for all metals except (cadmium, selenium, and zinc), are not available in the literature. For cadmium, selenium, and zinc, U.S. EPA (1995a) cited Ba values that were derived by

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dividing uptake slopes [(g COPC/kg DW tissue)/(g COPC/kg DW feed)], obtained from U.S. EPA (1992b), by a daily consumption rate of 0.2 kilograms DW per day by chicken. To obtain values reported in this HHRAP, the dry weight Ba value was converted to a fresh weight value by assuming a moisture content of 75 percent in eggs and chicken (U.S. EPA 1997h; and Pennington 1994).

**Mercuric Compounds** Elemental mercury is assumed to neither deposit onto soils nor get transferred to the aboveground plant parts or grains. Therefore, there is no transfer of elemental mercury into the animal tissue. Therefore, Ba values for elemental mercury are reported in this HHRAP as not applicable. This is based on the assumptions made regarding speciation and fate and transport of mercury from stack emissions.

If field data suggests otherwise, $Ba_{chicken}$ and Ba_{egg} values for elemental mercury can be derived from the uptake slope factors as provided in U.S. EPA (1992b) and U.S. EPA (1995a), using the same consumption rates discussed earlier for metals like cadmium, selenium, and zinc.

$Ba_{chicken}$ and Ba_{egg} values reported in this HHRAP for mercuric chloride and methyl mercury were derived from data in U.S. EPA (1997g). U.S. EPA (1997g) provided $Ba_{chicken}$ and Ba_{egg} values for mercury, but did not specify for which form of mercury. Consistent with U.S. EPA (1997g), mercury is assumed to be speciate into 87 percent divalent mercury and 13 percent methyl mercury in herbivore animal tissue. Also, assuming that the $Ba_{chicken}$ and Ba_{egg} values provided in U.S. EPA (1997g) were for total mercury in animal tissue, then biotransfer factors in U.S. EPA (1997g) can be apportioned in the fractions it is assumed to be found in animal tissue.

Therefore, values reported in this HHRAP are based on the following:

- Default $Ba_{chicken}$ value of 0.11 day/kg DW for mercury obtained from U.S. EPA (1997g) was converted to a fresh weight basis assuming a 75 percent moisture content in chicken (U.S. EPA 1997h; and Pennington 1994). The calculated $Ba_{chicken}$ (fresh weight) value was multiplied by (1) 0.13 to obtain a value for methyl mercury, and (2) 0.87 to obtain a value for mercuric chloride (divalent mercury).

- Default Ba_{egg} value of 0.11 day/kg DW for mercury obtained from U.S. EPA (1997g) was converted to a fresh weight basis assuming a 75 percent moisture content in eggs (U.S. EPA 1997h; and Pennington 1994). The calculated Ba_{egg} (fresh weight) value was multiplied by (1) 0.13 to obtain a value for methyl mercury, and (2) 0.87 to obtain a value for mercuric chloride (divalent mercury).

A3.5.4 Bioconcentration and Bioaccumulation Factors for Fish

Bioconcentration and bioaccumulation factors for fish are used for various compounds, depending on the K_{ow} value of the organic compound. Bioconcentration factors for fish (BCF_{fish}) were used for organics (except PCDDs, PCDFs, and PCBs) with a log K_{ow} value less than 4.0; and for metals (except lead and mercury). Bioaccumulation factors for fish (BAF_{fish}) were used for organics (except PCDDs, PCDFs, and PCBs) with a log K_{ow} value greater than 4.0, lead, and mercuric compounds. Biota-sediment accumulation factors for fish ($BSAF_{fish}$) were used for PCDDs, PCDFs, and PCBs.

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A3.5.4.1   Bioconcentration Factors for Fish (BCF_{fish})

BCF_{fish} is the ratio of the COPC concentration in fish to the COPC concentration in the water column where the fish is exposed. It accounts for uptake of COPCs by fish from water passing across the gills. BCF values for fish were used for all organic compounds with a log K_{ow} of less than 4.0 (cutoff value with BAF_{fish}) and for all metals, except lead and mercury, as cited in U.S. EPA (1995b). This implies that the concentration of COPC in the fish is only due to water intake by the fish, and compounds with a log K_{ow} of less than 4.0 are assumed not to bioaccumulate.

BCF values reported in this HHRAP are either:

1)   Geometric mean of a valid number of field-measured values obtained from various field studies (or)

2)   Geometric mean of laboratory-measured values obtained from various experimental studies (or)

3)   Estimated values calculated using a correlation equation

NOTE: When only one valid field-measured value for a COPC was found in the literature, the higher of the field-measured value and the geometric mean of laboratory-measured values, was used.

In general, field measured BCFs were assumed to be based on total (dissolved and suspended) water column concentrations; and laboratory measured BCFs were assumed to be based on dissolved water column concentrations. This distinction is important for compounds with a log K_{ow} of greater than or equal to 4.0, because significant amounts of a COPC can partition into the suspended sediment organic carbon (or particulate phase) of the water column. For compounds with a log K_{ow} of less than 4.0, most of COPC is associated with the dissolved phase of the water column and negligible amounts of COPC is associated with the suspended sediment phase in the water column. Therefore, for compounds with a log K_{ow} of less than 4.0, BCF values based on dissolved COPC water concentrations in the water column are essentially the same as BCF values based on total (dissolved + suspended) COPC water concentrations in the water column.

This HHRAP does not recognize differences in total versus dissolved water concentrations when calculating fish concentrations from BCF_{fish} values for compounds with a log K_{ow} of less than 4.0. Since, dissolved water concentrations is the major contributing factor from compounds with a log K_{ow} of less than 4.0, all BCF_{fish} values (irrespective of whether they were derived using total or dissolved water concentrations) can be multiplied by COPC concentration in the dissolved water column (C_{dw}) to calculate fish concentrations. This assumption is necessary because (1) literature data is often unclear if the water concentrations are dissolved or total concentrations, and (2) most of the literature reviewed indicated that laboratory experiments were conducted using filtered or distilled water; or the experiments were conducted using fresh water, but were filtered before analyses for water concentrations.

Organics For organics with a log K_{ow} value of less than 4.0, BCF_{fish} values were obtained from either of two methods:

•   Field-measured or laboratory-measured values from various experimental studies were evaluated by U.S. EPA (1998). This information is summarized in the following document:

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U.S. EPA. 1998. *Screening Level Ecological Risk Assessment Protocol for Hazardous Waste Combustion Facilities.* Draft Interim Final. April.

Field-measured data is only (1) available for a limited number of compounds, and (2) based on a single study. In such cases, the field-measured value or the geometric mean of field-measured values were compared with the geometric mean of laboratory-measured values, and the higher one used. A detailed discussion on sources of BCF values and methodology followed are provided in Appendix C of U.S. EPA (1998).

- When measured values were not available or could not be evaluated, the following correlation equation recommended by Lyman, Reehl, and Rosenblatt (1982) was used:

$$\log BCF_{fish} = -0.23 + 0.76 \log K_{ow} \qquad \text{Equation A-3-19}$$

Correlation Equation A-3-19 was developed by the following:

- Veith, G.D., K.J. Macek, S.R. Petrocelli, and J. Caroll. 1980. "An Evaluation of Using Partition Coefficients and Water Solubility to Estimate Bioconcentration Factors for Organic Chemicals in Fish." *Journal of Fish. Res. Board Can.* Prepublication Copy.

Veith, Macek, Petrocelli, and Caroll (1980) measured *BCF* values for four fish species in flow-through laboratory studies that were exposed to a wide range of organic chemicals. BCF_{fish} values calculated by using correlation Equation A-3-19 are (1) based on dissolved water concentrations, and (2) not lipid-normalized.

BCF_{fish} values provided in U.S. EPA (1995b) were either measured or calculated values. For BCF_{fish} values, U.S. EPA (1995b) either (1) obtained measured values from various literature sources U.S. EPA's AQUIRE database, or (2) used empirical chemical class-specific correlation equations. U.S. EPA (1998) reviewed a lot of original literature sources cited by the AQUIRE database. In general, BCF values in the AQUIRE database were either reported wrong, incorrectly calculated, or calculated from invalid data. U.S. EPA (1995b) also specified that the BCF values were lipid-normalized. Therefore, BCF_{fish} values could not be used in this HHRAP.

U.S. EPA (1994f) and NC DEHNR (1997) estimated BCF_{fish} values for PAHs and pesticides using correlation equations provided in the following:

- Ogata, M., K. Fujisawa, Y. Ogino, and E. Mano. 1984. "Partition Coefficients as Measure of Bioconcentration Potential of Crude Oil Compounds in Fish and Shellfish." *Bulletin of Environmental COPC Toxicology.* Volume 33. Page 561.

- Ellegehausen, H., J.A. Guth, and H.O. Esser. 1980. "Factors Determining the Bioaccumulation Potential of Pesticides in the Individual Compartments of Aquatic Food Chains." *Ecotoxicology and Environmental Safety.* 4:134.

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However, because of the limited applicability to only specific classes of compounds (PAHs and pesticides), values from U.S. EPA (1994f) and NC DEHNR (1997) were not used in this HHRAP.

U.S. EPA (1994f) and NC DEHNR (1997), both used a log K_{ow} cutoff value of 5.5, which implies that (1) for a log K_{ow} of less than 5.5, BCFs for fish were used, and (2) for a log K_{ow} of greater than 5.5, BAFs for fish were used. U.S. EPA (1995b) stated that a cutoff value of 4.0 is more widely accepted by the scientific community, based on experimental results.

Therefore, for consistency, BCF_{fish} values for this HHRAP, were obtained from experimental field and laboratory studies when available. When measured values were not available, values were calculated using correlation Equation A-3-19.

Metals For metals (except lead and mercury), BCF_{fish} values reported in this HHRAP are measured values obtained from various literature studies, as cited in U.S. EPA (1998). Measured values from various experimental studies were evaluated by U.S. EPA (1998). Detailed discussion and sources of measured values were provided in U.S. EPA (1998). For lead, a BAF is more applicable than a BCF as it tends to bioaccumulate. The BAF value for lead is discussed in Section A3.4.4.2.

Mercuric Compounds For mercuric compounds, a BAF is more applicable than a BCF as they tend to bioaccumulate. BAF values for the mercuric compounds are discussed in the following Section A3.4.4.2.

A3.5.4.2   Bioaccumulation Factors for Fish (BAF_{fish})

BAF_{fish} is the ratio of the COPC concentration in fish to the COPC concentration in the water body where the fish are exposed. The BAF_{fish} accounts for uptake of COPCs by fish from water and sediments passing across the gills, and from consumption of various foods including plankton, daphnids, and other fish. BAFs for fish were used for organic compounds (except PCBs, PCDDs, and PCDFs) with a log K_{ow} greater than 4.0, lead and mercuric compounds.

For compounds with a log K_{ow} of greater than or equal to 4.0, COPCs can significantly partition into the suspended sediment organic carbon (or particulate phase) of the water column. Therefore, BAF values should be based on total (dissolved and suspended) water column concentrations. BAFs reported in this HHRAP are either:

1)   Geometric mean of field-measured values obtained from various experimental studies (or)
2)   Predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured BCFs. A FCM is the ratio of a BAF to a BCF, and is used to account for food chain biomagnification from a lower to a upper trophic level (or)
3)   Predicted values calculated by multiplying a FCM with an estimated BCF. BCFs were estimated using correlation Equation A-3-19.

NOTE: When only one valid field-measured value for a COPC was found in the literature, the higher of the field-measured value and the geometric mean of laboratory-measured values, was used.

In general, (1) field-measured BAFs were assumed to be based on total (dissolved and suspended) water column concentrations, (2) laboratory-measured BCFs, and therefore, the BAFs predicted from them, were

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assumed to be based on dissolved water column concentrations, and (3) estimated BCFs using correlation Equation A-3-19, and therefore, the BAFs predicted from them, were assumed to be based on dissolved water column concentrations. In addition, field-measured BCFs, for compounds with a log K_{ow} greater than 4.0, were assumed to be equal to BAFs, because the tissue concentrations are a result of uptake of water (dissolved and suspended), sediment, and various trophic level food.

For consistency, all field-measured BAF (or BCF) values were adjusted according to the methodology specified in U.S. EPA (1995bc) to include only the dissolved water column fractions; (i.e., the BAFs based on total water concentrations were converted to BAFs based on dissolved water concentrations). This was done, so that all BAF_{fish} values (based on dissolved water concentrations) can be multiplied by the COPC concentration in the dissolved water column (C_{dw}) to calculate fish concentrations.

In U.S. EPA (1995b), BAF values were estimated based on the models developed for the limnetic ecosystem by the following:

- Thomann, R.V. 1989. "Bioaccumulation Model of Organic Chemical Distribution in Aquatic Food Chains." *Environmental Science and Technology.* 23(6):699-707.

and, for the littoral ecosystem by the following:

- Thomann, R.V., J.P. Connolly, and T.F. Parkerton. 1992. "An Equilibrium Model of Organic Chemical Accumulation in Aquatic Food Webs with Sediment Interaction." *Environmental Toxicology and Chemistry.* 11:615-629.

BAF values were predicted by multiplying a laboratory-measured or predicted BCF by a FCM. The Thomann (1989) and Thomann, Connolly, and Parkerton (1992) models were adopted by U.S. EPA, Office of Water, for the Great Lakes Water Quality Initiative in 1993. In 1995, U.S. EPA, Office of Water, developed BAFs based on the following study:

- Gobas, F.A.P.C. 1993. "A Model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: application to Lake Ontario." Ecological Modelling. 69:1-17.

The Gobas (1993) model was adopted to develop the latest water quality criteria and is provided in the following two documents:

- U.S. EPA. 1995bb. *Water Quality Guidance for the Great Lakes System. Supplementary Information Document.* Office of Water. EPA-820-B-95-001. March.

- U.S. EPA. 1995bc. *Great Lakes Water Quality Initiative. Technical Support Document for the Procedure to Determine Bioaccumulation Factors.* Office of Water. EPA-820-B-95-005. March.

The Gobas (1993) food-chain model was preferred because, unlike the Thomann (1989) model, it includes both benthic and pelagic food chains, thereby estimating exposure of organisms to compounds from both the sediment and the water column. Other inherent drawbacks of the Thomann (1989) model were that the model: (1) did not take into account metabolism, biotransformation, degradation, persistence, or seasonal or temporal variability, (2) is extremely sensitive to certain input parameter such as the lipid content,

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(3) incorrectly adopted FCMs, (4) is questionable in its assumption that the system is at steady state or in equilibrium, and (5) had little application for compounds with a log K_{ow} greater than 6.5, because the sediment route of exposure was not considered.

The Gobas (1993) model: (1) accounts for metabolism, but sets the metabolic rate to zero because of lack of data for individual compounds, (i.e., the metabolism is assumed not to occur), (2) incorporates the concentration of the compound in both the sediment and the water column, the sediment route being especially useful for compounds with a log K_{ow} greater than 6.5, and (3) includes the disequilibrium between concentrations of the compounds in sediment and the water column. Although the Thomann, Connolly, and Parkerton (1992) model accounts for sediment interaction, according to U.S. EPA (1995bb), the Gobas (1993) model required fewer input parameters which could be more easily specified.

Therefore, this HHRAP recommends BAF values derived from the Gobas (1993) model. The methodology to derive BAF values using BCFs and a FCM is described in detail in U.S. EPA (1995bc).

The following equation cited in U.S. EPA (1995bc) was used to convert the BAF based on total water concentrations to a BAF based on dissolved water concentrations:

$$ f_{fd} = \frac{1}{1 + \frac{(DOC)\ (K_{ow})}{10} + (POC)\ (K_{ow})} $$

Equation A-3-20

where

f_{fd} = fraction of COPC that is freely dissolved in water
DOC = concentration of dissolved organic carbon, kg organic carbon / L water
POC = concentration of particulate organic carbon, kg organic carbon / L water

Since, the Gobas (1993) model was derived from a study conducted at Lake Ontario, DOC and POC values for Lake Ontario were used. Values cited in U.S. EPA (1995bc) were:

DOC = 2×10^{-6} kg/L
POC = 7.5×10^{-9} kg/L

A BAF based on dissolved water concentrations can be calculated from a BAF based on total water concentrations as follows:

$$ BAF\ (dissolved) = \frac{BAF\ (total)}{f_{fd}} - 1 $$

Equation A-3-21

FCMs were obtained from Table 2 of U.S. EPA (1995bc). U.S. EPA (1995bc) provided FCMs as a function of log K_{ow} in increments of 0.1 for trophic level 2, 3, and 4 aquatic organisms. For this HHRAP, humans are assumed to consume trophic level 3 or 4 fish. The higher FCM value of trophic levels 3 and 4 was used in this HHRAP. When the log K_{ow} value of a COPC in this HHRAP was between two log K_{ow}

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values listed in Table 2 of U.S. EPA (1995bc), the FCM for the next highest log K_{ow} value was used.

__Organics__ For all organics (except PCBs, PCDDs and PCDFs) with a log K_{ow} greater than or equal to 4.0, the FCM, which accounts for accumulation through the food chain in addition to water, becomes greater than 1. Therefore, a BAF_{fish}, which takes the food chain into consideration, is more appropriate than a BCF_{fish}.

For all organics with a log K_{ow} greater than or equal to 4.0, BAFs were derived using one of following three methods:

1)	BAF =	Field measured BAF or BCF, adjusted for dissolved water concentrations
2)	BAF =	Laboratory measured BCF multiplied by a FCM for either trophic level 3 or 4 fish
3)	BAF =	Estimated BCF calculated using correlation equation A-3-19 multiplied by a FCM for either trophic level 3 or 4 fish

Both field and laboratory measured values were derived from various literature sources cited in U.S. EPA (1998). FCMs were obtained from U.S. EPA (1995bc).

BAF values in U.S. EPA (1995b) were either (1) derived from the Thomann (1989) and Thomann, Connolly, and Parkerton (1992) models for organics with a log K_{ow} less than 6.5 , or (2) assumed a default BAF_{fish} value of 1,000 for organics with a log K_{ow} greater than 6.5. The default value was based on (1) an analysis of available data on PAHs, and (2) recommendations by the following:

- Stephan, C.E., and others. 1993. "Derivation of Proposed Human Health and Wildlife Bioaccumulation Factors for the Great Lakes Initiative." Office of Research and Development, U.S. Environmental Research Laboratory. PB93-154672. Springfield, Virginia.

U.S. EPA (1994f) presented BAF_{fish} values estimated by three different methods: (1) measured BAF_{fish}, (2) measured BCF_{fish} multiplied by a food-chain multiplier estimated from log K_{ow}, and (3) BAF_{fish} estimated from log K_{ow}. However, it provides values for only six compounds.

NC DEHNR (1997) provided BAF_{fish} values without any references specific to sources of values for each compound. U.S. EPA (1994f) and NC DEHNR (1997) both used a log K_{ow} cutoff value of 5.5, which implies that accumulation occurs only at a log K_{ow} greater than 5.5. U.S. EPA (1995b) stated that a cutoff value of 4.0 is more widely accepted by the scientific community. Therefore, BAF_{fish} values in the primary guidance documents were not used in this HHRAP.

__Metals (lead)__ For lead, the food-chain multiplier becomes greater than 1; therefore, a BAF is more appropriate. The BAF_{fish} value reported in this HHRAP for lead was obtained as a geometric mean from various literature sources described in U.S. EPA (1998). Since metals are assumed insoluble under neutral conditions, the dissolved and total water concentrations are almost equal. However, for consistency, the BAF_{fish} value for lead was adjusted for dissolved fractions.

__Mercuric Compounds__ Consistent with U.S. EPA (1997g), elemental mercury is expected not to deposit significantly onto soils and surface water. Therefore, there it is assumed that there is no transfer of elemental mercury into fish. Fish are assumed to be exposed only to the divalent and organic forms of

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mercury that exists in the water and soil/sediment media. However, consistent with the conservative approach adopted by previous guidance documents, all of mercury in the fish is assumed to exist or be converted to the methyl mercury (organic) form after uptake into the fish tissue. Therefore, for this HHRAP, the BAF_{fish} value for methyl mercury was obtained from U.S. EPA (1997g) for a trophic level 4 fish.

A3.5.4.3   Biota-Sediment Accumulation Factor for Fish ($BSAF_{fish}$)

PCDDs, PCDFs, and PCBs   For PCDDs, PCDFs, and PCBs, $BSAF_{fish}$ values should be used instead of BAFs for fish. $BSAF_{fish}$ values reported in this HHRAP were obtained from U.S. EPA (1994a).

$BSAF_{fish}$ accounts for the transfer of COPCs from the bottom sediment to the lipid in fish. U.S. EPA (1994a) and (1993d) recommended using $BSAF_{fish}$ values for dioxin-like compounds, including PCBs, because of their lipophilic nature. U.S. EPA (1995b) also stated that $BSAF_{fish}$ values (1) were used for 2,3,7,8-TCDD and PCBs to estimate protective sediment concentrations instead of surface water concentrations, and (2) were a more reliable measure of bioaccumulation potential because of the analytical difficulties in measuring dissolved concentrations in surface water. $BSAF$ values in the literature vary because of the different experimental and sampling techniques used. U.S. EPA (1994a) provided exposure scenarios for conducting site-specific assessments to dioxin-like compounds. For each scenario, U.S. EPA (1994a) recommended the use of the following $BSAF_{fish}$ values based on the amount of chlorination of the PCDD or PCDF:

- For TetraCDDs and TetraCDFs, $BSAF_{fish} = 9.0 \times 10^{-02}$

- For TetraCDDs and TetraCDFs, $BSAF_{fish} = 9.0 \times 10^{-02}$

- For TetraCDDs and TetraCDFs, $BSAF_{fish} = 4.0 \times 10^{-02}$

- For TetraCDDs and TetraCDFs, $BSAF_{fish} = 5.0 \times 10^{-03}$

- For TetraCDDs and TetraCDFs, $BSAF_{fish} = 1.0 \times 10^{-04}$

Homologue group $BSAF_{fish}$ values obtained from U.S. EPA (1994a) were either measured or estimated values that were based on a whole fish lipid content of 7 percent and an organic carbon content of 3 percent. The $BSAF_{fish}$ values reported in this HHRAP are consistent with the values presented in primary guidance documents.

A3.6   HUMAN HEALTH BENCHMARKS

The following sections discuss carcinogenic and noncarcinogenic toxicity benchmarks of compounds. The toxicity information provided in the HHRAP is for informational purposes to help permitting authorities explain the basis for selecting contaminants of concern. Since toxicity benchmarks and slope factors may change as additional toxicity research is conducted, permitting authorities should consult with the most current version of EPA's Integrated Risk Information System (IRIS) and *Health Effects Assessment Summary Tables* before completing a risk assessment to ensure that the toxicity data used in the risk assessment is based upon the most current Agency consensus.

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A3.6.1 Reference Dose (*Rfd*) and Reference Concentration (*RfC*)

Reference dose (*Rfd*) is defined as a daily intake rate of a compound estimated to pose no appreciable risk of deleterious effects over a specific exposure duration (U.S. EPA 1989e). Reference concentration (*Rfc*) is defined as the concentration of a compound estimated (with uncertainty spanning perhaps an order of magnitude) to pose no appreciable risk of deleterious effects over a specific exposure duration (U.S. EPA 1989e).

The reference dose (*Rfd*) and reference concentration (*RfC*) values for all compounds were obtained from one of the following references (listed in order of preference):

- U.S. EPA. 1997b. *Integrated Risk Information System (IRIS)*. June - December.

- U.S. EPA. 1995c. "Health Effects Assessment Summary Tables (HEAST)." Fiscal Year Annual 1995. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/036.

- U.S. EPA. 1997c. "Health Effects Assessment Summary Tables (HEAST)." Fiscal Year Annual 1997. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/036.

- U.S. EPA. 1997d,e,f. " Risk Assessment Issue Papers". Superfund Technical Support Center. National Center for Environmental Assessement. December.

- U.S. EPA. 1997a. "Risk-Based Concentrations." Region 3. June

- U.S. EPA. 1996c. "Region 9 Preliminary Remediation Goals." Region 9. August.

The U.S. EPA (1997b) IRIS database and the U.S. EPA (1995c, 1997c) HEAST are compilations of human health risk information obtained from several literature sources. U.S. EPA (1995c, 1997c) cited IRIS as the main source of human health risk information.

Rfd and *RfC* values in this HHRAP were revised, because values in U.S. EPA (1997b) and U.S. EPA (1995c, 1997c) are updated regularly on the basis of literature data.

A3.6.2 Oral Cancer Slope Factor (*CSF*), *Inhalation CSF*, and *Inhalation Unit Risk Factor (URF)*

Oral CSF, inhalation CSF, and *inhalation URF* values for all compounds were obtained from U.S. EPA (1997b) or (1995c, 1997c). In addition, U.S. EPA (1996c; 1997a,d,e,f) were also used to obtained the *oral CSF, inhalation CSF*, and the *inhalation URF* when these values were not available in U.S. EPA (1997b) or (1995c; 1997c). Additional guidance for determining reference concentrations for chronic inhalation exposure is provided in U.S. EPA (1994h).

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A3.6.3   Explanation of Calculated Toxicity Benchmark Values

The preference for health benchmarks is to obtain values from IRIS or HEAST. The following methodology was used to calculate missing benchmarks using available benchmarks that are based on route-to-route extrapolation:

1) *Oral RfDs* presented in IRIS/Heast/EPA reviewed documents were used if available. Missing oral *RfDs* were calculated from the *RfC* assuming route-to-route extrapolation using the following equation:

$$Oral\ RfD = \frac{RfC \cdot 20\ m^3/d}{70\ kg\ BW}$$

2) *Oral CSFs* presented in IRIS/Heast/EPA reviewed documents were used when available. In the case of missing Oral CSFs:

   a) *Oral CSF = Inhalation CSF*, or

   b) *Oral CSF = Inhalation CSF* calculated from Inhalation URF assuming route-to-route extrapolation.

3) *Inhalation RfCs* presented in IRIS/Heast/EPA reviewed documents were used when available. If *RfCs* were not available they were calculated from the *RfD* assuming route-to-route extrapolation using the following equation:

$$Inhalation\ RfC = \frac{RfD \cdot 70\ kg\ BW}{20\ m^3/d}$$

4) *Inhalation RfD_i* values were calculated as follows:

   a) From the *inhalation RfC* obtained from IRIS/Heast/EPA reviewed documents using the following equation:

$$RfD_{inh} = \frac{RfC \cdot 20\ m^3/d}{70\ kg}$$

   b) If the *RfC* was not available from IRIS/Heast/EPA reviewed documents, the following was assumed:

$$Inhalation\ RfD = Oral\ RfD$$

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5) For *inhalation URF*s, values were obtained from IRIS/Heast/EPA reviewed documents. If the *inhalation URF*s were not available they were calculated from *oral CSF*, using the following equation:

$$Inhal.\ URF = \frac{Inhal.\ URF \cdot 20\ m^3/d}{70\ kg \times 1000\ \mu g/mg}$$

6) The *inhalation CSF*s presented in IRIS/Heast/EPA reviewed documents were used when available.

   a) If no *inhalation CSF* was available; it was calculated from *inhalation URF*, using the following equation:

$$Inhal.\ CSF = \frac{Inhal.\ URF \cdot 70\ kg}{20\ m^3/d} \times 1000\ \mu g/mg$$

   b) If no *inhalation URF* was available; the following was assumed based on route-to-route extrapolation:

$$Inhalation\ CSF = Oral\ CSF$$

A3.6.4 Uncertainties Involved when using Toxicity Benchmarks Calculated based on Route-to-Route Extrapolation

In the assessment of noncarcinogenic and carcinogenic risk from COPCs, EPA-derived or reviewed health benchmarks (*RfD*s, *RfC*s, *CSF*s, *URF*s, and *Inhalation CSF*s) are recommended. However, for numerous compounds, a complete set of inhalation and oral EPA-derived health benchmarks are not available. In such cases, for this HHRAP, the health benchmarks were calculated based on available EPA-derived benchmarks values. For instance, if the *oral RfD* (mg/kg/day) was available and the *RfC* (mg/m^3) was not; the *RfC* was calculated by multiplying the *RfD* by an average human inhalation rate of 20 m^3/day and dividing by the average human body weight of 70 kg. This conversion is based on a route-to-route extrapolation, which assumes that the toxicity of the given chemical is equivalent over all routes of exposure.

This process does introduce uncertainty into the risk assessment. By using this method, the risk assessor must assume that the qualitative data supporting the benchmark value for a certain route also applies to the route in question. For example, if an *RfD* is available and the *RfC* is calculated from that value, the risk assessor is assuming that the toxicity seen following oral exposure will be equivalent to toxicity following inhalation exposure. This assumption could overestimate or underestimate the toxicity of the given chemical following inhalation exposure.

Because of the degree of uncertainty involved in using toxicity benchmark values calculated based on route-to-route extrapolation, this HHRAP recommends that a qualitative assessment of the toxicity information available for the chemical and exposure route be performed. This will enable the risk

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assessor to make a well informed decision concerning the validity of values calculated based on route-to-route extrapolation. This qualitative assessment should also be included in the uncertainty section of the risk assessment.

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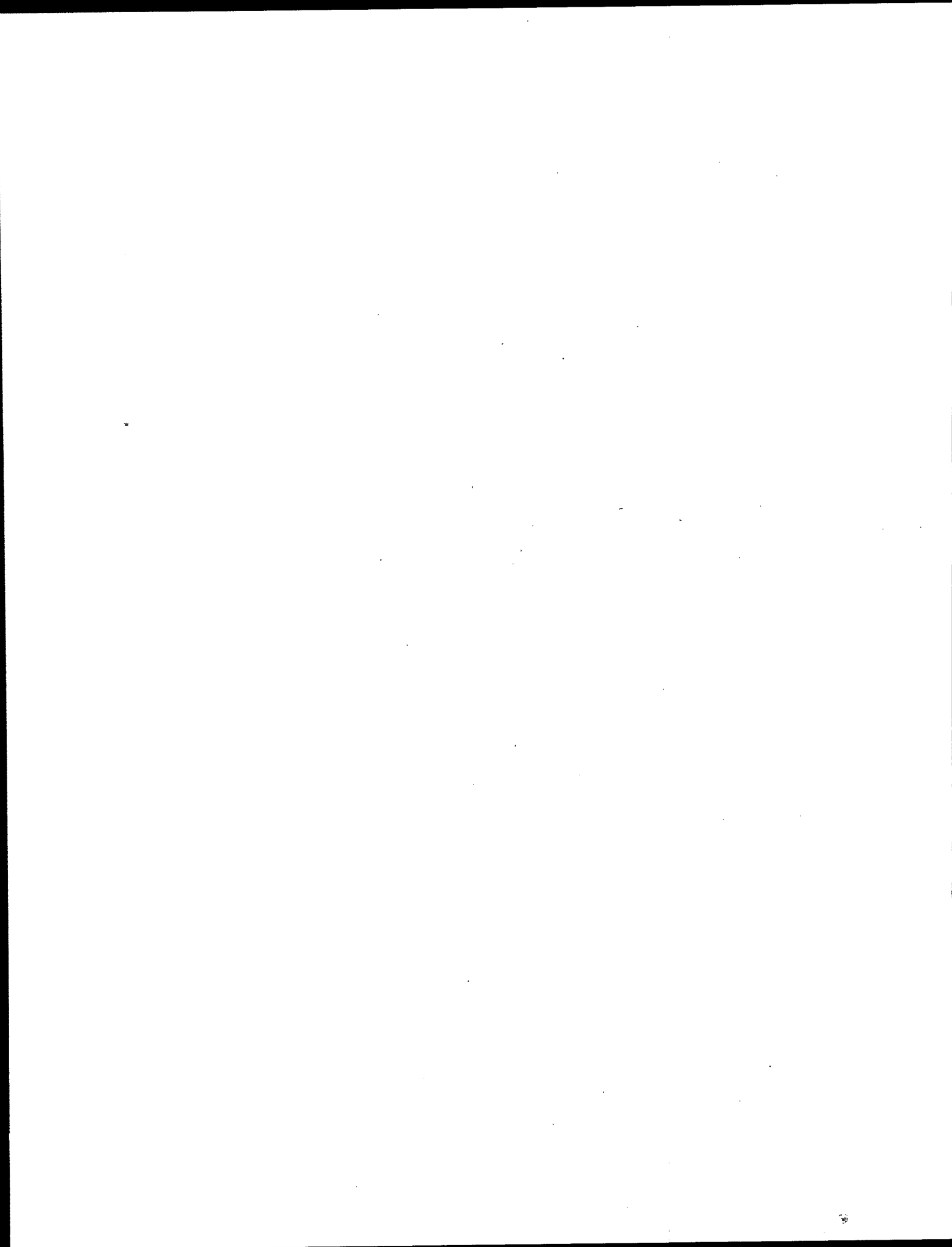
Agency for Toxic Substances and Disease Registry (ATSDR). 1987. *Draft Toxicological Profile for Di(2-ethylhexyl) Phthatlate.* Oak Ridge National Laboratory. December.

Bacci E., D. Calamari, C. Gaggi, and M. Vighi. 1990. "Bioconcentration of Organic Chemical Vapors in Plant Leaves: Experimental Measurements and Correlation." *Environmental Science and Technology.* Volume 24. Number 6. Pages 885-889.

Bacci E., M. Cerejeira, C. Gaggi, G. Chemello, D. Calamari, and M. Vighi. 1992. "Chlorinated Dioxins: Volatilization from Soils and Bioconcentration in Plant Leaves." *Bulletin of Environmental Contamination and Toxicology.* Volume 48. Pages 401-408.

Baes, C.F. 1982. "Prediction of Radionuclide K_d values from Soil-Plant Concentration Ratios." *Tran. American Nuclear Society.* 41:53-54.

Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. "Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides through Agriculture." Oak Ridge National Laboratory. Oak Ridge, Tennessee.

Banerjee, S., P.H. Howard, and S.S. Lande. 1990. "General Structure Vapor Pressure Relationships for Organics." *Chemosphere.* 21(10-11). Pages 1173-1180.

Belcher, G.D., and C.C. Travis. 1989. "Modeling Support for the RURA and Municipal Waste Combustion Projects: Final Report on Sensitivity and Uncertainty Analysis for the Terrestrial Food Chain Model." Interagency Agreement No. 1824-A020-A1. Office of Risk Analysis, Health and Safety Research Division. Oak Ridge National Laboratory. Oak Ridge, Tennessee. October.

Bidleman, T.F. 1984. "Estimation of Vapor Pressures for Nonpolar Organic Compounds by Capillary Gas Chromatography. *Analytical Chemistry.* Volume 56. Pages 2490-2496.

Bidleman, T.F. 1988. "Atmospheric Processes." *Environmental Science and Technology.* Volume 22. Number 4. Pages 361-367.

Billington, J.W., G. Huang, F. Szeto, W.Y. Shiu, and D. Mackay. 1988. "Preparation of Aqueous Solutions of Sparingly Soluble Organic Substances: I. Single Component Systems." *Environmental Toxicology and Chemistry.* Volume 7. Pages 117-124.

Briggs, G.G., R.H. Bromilow, and A.A. Evans. 1982. "Relationships Between Lipophilicity and Root Uptake and Translocation of Nonionized Chemicals by Barley." *Pesticide Science.* Volume 13. Pages 495-504.

Bruggeman, W.A., J. Van Der Steen, and O. Hutzinger. 1982. "Reversed-Phase Thin-Layer Chromatography of Polynuclear Aromatic Hydrocarbons and Chlorinated Biphenyls. Relationship

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with Hydrophobicity as Measured by Aqueous Solubility and Octanol-Water Partition Coefficient." *Journal of Chromatography.* Volume 238. Pages 335-346.

Budavari, S., M.J. O'Neil, A. Smith, and P.E. Heckelman. 1989. *The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals.* 11th Edition. Merck and Company, Inc. Rahway, New Jersey.

California Environmental Protection Agency (CEPA). 1993. "Parameter Values and Ranges for CALTOX." Draft. Office of Scientific Affairs. California Department of Toxic Substances Control. Sacramento, CA. July.

Chamberlain, A.C. 1970. "Interception and Retention of Radioactive Aerosols by Vegetation." *Atmospheric Environment.* Pergamon Press. Great Britain. Volume 4. Pages 57-78.

Di Toro, D.M. 1985. "A Particle Interaction Model of Reversible Organic Chemical Sorption." *Chemosphere.* 14(10):1503-1538.

DiToro, D.M., C.S. Zarba, D.J. Hansen, W.J. Berry, R.C. Swartz, C.E. Cowan, S.P. Pavlou, H.E. Allen, N.A. Thomas, and P.R. Paquin. 1991. "Technical Basis for Establishing Sediment Quality Criteria for Nonionic Compounds Using Equilibrium Partitioning." *Environmental Toxicology and Chemistry.* 10:1541-1583.

Eadie, B.J., N.R. Morehead, and P.F. Landrum. 1990. "Three-Phase Partitioning of Hydrophobic Organic Compounds in Great Lakes Waters." *Chemosphere.* Volume 20. Pages 161-178.

Ellegehausen, H., J.A. Guth, and H.O. Esser. 1980. "Factors Determining the Bioaccumulation Potential of Pesticides in the Individual Compartments of Aquatic Food Chains." *Ecotoxicology and Environmental Safety.* 4:134.

Gobas, F.A.P.C. 1993. "A Model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: application to Lake Ontario." Ecological Modelling. 69:1-17.

Hansch, C., and A. Leo. 1985. *Medchem Project.* Pomona College. Clairemont, California. Issue No. 26.

Haque, R., and D. Schmedding. 1975. "A Method of Measuring the Water Solubility of Hydrophobic Chemicals: Solubility of Five Polychlorinated Biphenyls." *Bulletin of Environmental Contamination and Toxicology.* Volume 14. Pages 13-18.

Hinckley, D.A., T.F. Bidleman, and W.T. Foreman. 1990. "Determination of Vapor Pressures for Nonpolar and Semipolar Organic Compounds from Gas Chromatographic Retention Data." *Journal of Chemical Engineering Data.* Volume 35. Pages 232-237.

Hoffman, F.O., K.M. Thiessen, M.L. Frank, and B.G. Blaylock. 1992. "Quantification of the Interception and Initial Retention of Radioactive Contaminants Deposited on Pasture Grass by Simulated Rain." *Atmospheric Environment.* 26A(18):3313-3321.

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Howard, P.H. 1989-1993. *Handbook of Environmental Fate and Exposure Data For Organic Chemicals. Volume I: Large Production and Priority Pollutants (1989). Volume II: Solvents (1990). Volume III: Pesticides (1991). Volume IV: Solvents2 (1993).* Lewis Publishers. Chelsea, Michigan.

Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan, and E.M. Michalenko, 1991. *Handbook of Environmental Degradation Rates.* Lewis Publishers. Chelsea, Michigan.

Junge, C. E. 1977. *Fate of Pollutants in the Air and Water Environments, Part I.* Suffet, I. H., Ed. Wiley. New York. Pages 7-26.

Karickhoff, S.W., D.S. Brown, and T.A. Scott. 1979. "Sorption of Hydrophobic Pollutants on Natural Sediments." *Water Resources.* 13:241-248.

Karickhoff, S.W., and J.M. Long. 1995. " Internal Report on Summary of Measured, Calculated, and Recommended Log K_{ow} Values." Environmental Research Laboratory. Athens, Georgia. April 10.

Landrum, P.F., S.R. Nihart, B.J. Eadie, and W.S. Gardner. 1984. "Reverse-Phase Separation Method for Determining Pollutant Binding to Aldrich Humic Acid and Dissolved Organic Carbon of Natural Waters." *Environmental Science and Technology.* 18(3):187-192.

Lorber, M. 1995. "Development of an Air-to-plant Vapor Phase Transfer for Dioxins and Furans. Presented at the 15th International Symposium on Chlorinated Dioxins and Related Compounds". August 21-25, 1995 in Edmonton, Canada. Abstract in *Organohalogen Compounds.* 24:179-186.

Lucius, J.E., R.O. Olhoeft, P.L. Hill, and S.K. Duke. 1992. *Properties and Hazards of 108 Selected Substances - 1992 Edition.* U.S. Department of the Interior Geological Survey. U.S. Geological Survey Open-File Report 92-527. September.

Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt. 1982. *Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds.* McGraw-Hill Book Company. New York, New York.

Ma, K.C., W.Y. Shiu, and D. Mackay. 1990. *A Critically Reviewed Compilation of Physical and Chemical and Persistence Data for 110 Selected EMPPL Substances.* Prepared for the Ontario Ministry of Environment. Water Resources Branch. Toronto, Ontario.

Mabey, W.R., J.H. Smith, R.T. Podoll, H.L. Johnson, H.L. Mill, T.W. Chiou, J. Gate, I. Waight-Partridge, H. Jaber, and D. Vanderberg. 1982. *Aquatic Fate Process Data for Organic Priority Pollutants.* U.S. EPA Report Number 440/4-81-014. December.

McCarthy, J.F., and B.D. Jimenez. 1985. "Interactions Between Polycyclic Aromatic Hydrocarbons and Dissolved Humic Material: Binding and Dissociation." *Environmental Science and Technology.* 19(11):1072-1076.

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Mackay, D., and S. Paterson. 1991. "Evaluating the Multimedia Fate of Organic Chemicals: A Level III Fugacity Model." *Environmental Science and Technology*. Volume 25(3). Pages 427-436.

Mackay, D., and W.Y. Shiu. 1975. "The Aqueous Solubility and Air-Water Exchange Characteristics of Hydrocarbons under Environmental Conditions." In *Chemistry and Physics of Aqueous Gas Solutions*. Electrochem. Soc., Inc. Princeton, New Jersey.

Mackay, D. W.Y. Shiu, and K.C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume I—Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Volume II—Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins, and Dibenzofurans. Volume III—Volatile Organic Chemicals*. Lewis Publishers. Chelsea, Michigan.

McLachlan, M.S., H. Thoma, M. Reissinger, and O. Hutzinger. 1990. "PCDD/F in an Agricultural Food Chain. Part I: PCDD/F Mass Balance of a Lactating Cow." *Chemosphere*. Volume 20 (Numbers 7-9). Pages 1013-1020.

Macrady, J.K., and S.P. Maggard. 1993. "Uptake and Photodegradation of 2,3,7,8-Tetrachlorodibenzo-p-dioxin Sorbed to Grass Foliage." *Environmental Science and Technology*. 27:343-350.

Mallon, B.J., and F.I. Harrison. 1984. "Octanol-Water Partitioning Coefficient of Benzo(a)pyrene: Measurement, Calculation, and Environmental Implications." *Bulletin of Environmental Contamination and Toxicology*. New York. Pages 316-323.

Miller, M.M., S.P. Wasik, G.L. Huang, W.Y. Shiu, and D. Mackay. 1985. "Relationships Between Octanol-Water Partition Coefficient and Aqueous Solubility." *Environmental Science and Technology*. 19(6):522-529.

Mills, W.B., J.D. Dean, D.B. Porcella, S.A. Gherini, R.J.M. Hudson, W.E. Frick, G.L. Rupp, and G.L. Bowie. 1982. *Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants*. Part 1. EPA 600/6-82-004a.

Montgomery, J.H., and L.M. Welkom. 1991. *Groundwater Chemicals Desk Reference*. Lewis Publishers. Chelsea, Michigan.

Murray, J.M., R.F. Pottie, and C. Pupp. 1974. "The Vapor Pressures and Enthalpies of Sublimation of Five Polycyclic Aromatic Hydrocarbons." *Can. J. Chem*. 52:557-563.

Moses, A.J. 1978. *The Practicing Scientist's Handbook. A Guide for Physical and Terrestrial Scientists and Engineers*. Van Nostrand Reinhold Company. New York, NY.

North Carolina Department of Environment, Health, and Natural Resources (NC DEHNR). 1997. *North Carolina Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

U.S. EPA Region 6
Multimedia Planning and Permitting Division
Center for Combustion Science and Engineering

U.S. EPA
Office of Solid Waste
A-3-46

Ogata, M., K. Fujisawa, Y. Ogino, and E. Mano. 1984. "Partition Coefficients as a Measure of Bioconcentration Potential of Crude Oil Compounds in Fish and Shellfish." *Bulletin of Environmental Contaminant Toxicology.* Volume 33. Page 561.

Pennington, J.A.T. 1994. *Food Value of Portions Commonly Used.* Sixteenth Edition. J.B. Lippincott Company, Philadelphia.

Research Triangle Institute (RTI). 1992. *Preliminary Soil Action Level for Superfund Sites, Draft Interim Report.* Prepared for U.S. Environmental Protection Agency (EPA) Hazardous Site Control Division, Remedial Operations Guidance Branch. Arlington, Virginia. EPA Contract No. 68-W1-0021. Work Assignment No. B-03. Work Assignment Manager, Loren Henning. December.

RTI. 1994. "Draft Report—Chemical Properties for Soil Screening Levels." North Carolina. July 26.

Smith, J.H., W.R. Mabey, N. Bahonos, B.R. Holt, S.S. Lee, T.W. Chou, D.C. Venberger, and T. Mill. 1978. *Environmental Pathways of Selected Chemicals in Fresh Water Systems: Part II, Laboratory Studies.* Interagency Energy-Environment Research Program Report. Environmental Research Laboratory. Office of Research and Development. U.S. EPA. Athens, Georgia. EPA-600/7-78-074. Page 304.

Stephenson, R.M., and S. Malanowski. 1987. *Handbook of the Thermodynamics of Organic Compounds.* Elsevier Publishing Company, Inc. New York.

Stephan, C.E., and others. 1993. "Derivation of Proposed Human Health and Wildlife Bioaccumulation Factors for the Great Lakes Initiative." Office of Research and Development, U.S. Environmental Research Laboratory. PB93-154672. Springfield, Virginia.

Stephens, R.D., M. Petreas, and G.H. Hayward. 1995. "Biotransfer and Bioaccumulation of Dioxins and Furans from Soil: Chickens as a Model for Foraging Animals." *The Science of the Total Environment.* 175: 253-273. July 20.

Thomann, R.V. 1989. "Bioaccumulation Model of Organic Chemical Distribution in Aquatic Food Chains." *Environmental Science and Technology.* 23(6):699-707.

Thomann, R.V., J.P. Connolly, and T.F. Parkerton. 1992. "An Equilibrium Model of Organic Chemical Accumulation in Aquatic Food Webs with Sediment Interaction." *Environmental Toxicology and Chemistry.* 11:615-629.

Thompson, S.E., C.A. Burton, D.J. Quinn, and Y.C. Ng. 1972. "Concentration Factors of Chemical Elements in Edible Aquatic Organisms." Lawrence Radiation Laboratory. Livermore, CA. UCRL-50564, Revision 1. (Reference cited in updated version of Chapman, W.H., H.L. Fisher, and M.W. Pratt. 1968).

Travis, C.C. and A.D. Arms. 1988. "Bioconcentration of Organics in Beef, Milk, and Vegetation." *Environmental Science and Technology.* 22:271-274.

U.S. EPA Region 6
Multimedia Planning and Permitting Division
Center for Combustion Science and Engineering

U.S. EPA
Office of Solid Waste
A-3-47

U.S. EPA. 1978. *Environmental Pathways of Selected Chemicals in Freshwater Systems: Part II. Laboratory Studies.* Interagency Energy-Environment Research and Development Program Report. Environmental Research Laboratory. Athens, GA. EPA 600/7-78-074. May.

U.S. EPA. 1986. *Superfund Public Health Evaluation Manual.* Office of Emergency and Remedial Response (OERR). Washington, D.C. October.

U.S. EPA. 1990. *Interim Final Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* EPA/600/6-90/003. January.

U.S. EPA. 1992a. *Handbook of Resource Conservation and Recovery Act (RCRA) Ground Water Monitoring Constituents: Chemical and Physical Properties.* EPA/530-R-92/022. Office of Solid Waste. Washington, D.C.

U.S. EPA. 1992b. *Technical Support Document for the Land Application of Sewage Sludge. Volumes I and II.* EPA 822/R-93-001a. Office of Water. Washington, D.C.

U.S. EPA. 1992c. *Risk Reduction Engineering Laboratory Treatability DataBase.* Version 5.0.

U.S. EPA. 1992d. *Estimating Exposure to Dioxin-Like Compounds.* Draft Report. Office of Research and Development. Washington, D.C. EPA/600/6-88/005B. August.

U.S. EPA. 1993a. *Assessment Tools for the Evaluation of Risk.*

U.S. EPA. 1993b. *Derivation of Proposed Human Health and Wildlife Bioaccumulation Factors for the Great Lakes Initiative.* Office of Research and Development, U.S. Environmental Research Laboratory. Duluth, Minnesota. March.

U.S. EPA. 1993c. "Proposed Water Quality Guidance for the Great Lakes System." *Federal Register.* 58:20802. April 16.

U.S. EPA. 1993d. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Office of Health and Environmental Assessment. Office of Research and Development. EPA-600-AP-93-003. November 10.

U.S. EPA. 1994a. *Estimating Exposure to Dioxin-Like Compounds.* Draft Report. Office of Research and Development. Washington, D.C. EPA/600/6-88/005Ca,b,c. June.

U.S. EPA. 1994b. *Superfund Chemical Data Matrix.* OERR. Washington, D.C. June.

U.S. EPA 1994c. *Draft Report-Chemical Properties for Soil Screening Levels.* Prepared for the OERR. Washington, DC. July 26.

U.S. EPA. 1994d. *CHEM8—Compound Properties Estimation and Data.* Version 1.00. CHEMDAT8 Air Emissions Program. Prepared for Chemicals and Petroleum Branch, OAQPS. Research Triangle Park. North Carolina. November 18.

U.S. EPA. 1994e. *Integrated Risk Information System.* December.

U.S. EPA Region 6   U.S. EPA
Multimedia Planning and Permitting Division   Office of Solid Waste
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U.S. EPA. 1994f. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes: Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* OERR. Office of Solid Waste. December 14.

U.S. EPA. 1994h. *Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry.* ORD. EPA/600/8-90/066F.

U.S. EPA. 1995a. *Memorandum regarding Further Studies for Modeling the Indirect Exposure Impacts from Combustor Emissions.* From Mathew Lorber, Exposure Assessment Group, and Glenn Rice, Indirect Exposure Team, Environmental Criteria and Assessment Office. Washington, D.C. January 20.

U.S. EPA. 1995b. *Review Draft Development of Human Health-Based and Ecologically-Based Exit Criteria for the Hazardous Waste Identification Project.* Volumes I and II. Office of Solid Waste. March 3.

U.S. EPA. 1995c. "Health Effects Assessment Summary Tables." Fiscal Year-1995 Annual. Office of Solid Waste and Emergency Response. Washington, D.C. EPA/540/R-95/036. May.

U.S. EPA. 1995d. *WATER8—Air Emissions Models Wastewater Treatment.* Version 4.0. OAQPS. Research Triangle Park. North Carolina. May 1.

U.S. EPA. 1995e. *Water Quality Guidance for the Great Lakes System. Supplementary Information Document.* Office of Water. EPA-820-B-95-001. March.

U.S. EPA. 1995f. *Great Lakes Water Quality Initiative. Technical Support Document for the Procedure to Determine Bioaccumulation Factors.* Office of Water. EPA-820-B-95-005. March.

U.S. EPA. 1996a. *Mercury Study Report to Congress. Volume III: An Assessment of Exposure from Anthropogenic Mercury Emissions in the United States.* SAB Review Draft. Office of Air Quality Planning and Standards and Office of Research and Development. EPA-452/R-96-001c. April.

U.S. EPA. 1996b. *Soil Screening Guidance: Technical Background Document and User's Guide.* Office of Solid Waste and Emergency Response. Washington, D.C. EPA/540/R-95/128. May.

U.S. EPA. 1996c. "Region 9 Preliminary Remediation Goals." Region 9. August.

U.S. EPA. 1997a. "Risk-Based Concentrations." Region 3. June

U.S. EPA. 1997b. *Integrated Risk Information System* (IRIS). June - December.

U.S. EPA. 1997c. "Health Effects Assessment Summary Tables (HEAST). Fiscal Year 1997 Update". Office of Solid Waste and Emergency Response. EPA-540-R-97-036. PB97-921199. July.

U.S. EPA Region 6   U.S. EPA
Multimedia Planning and Permitting Division   Office of Solid Waste
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U.S. EPA. 1997d. " Risk Assessment Issue Papers for: Derivation of a Provisional Chronic and Subchronic RfC for Chloromethane (CASRN 74-87-3)." Superfund Technical Support Center. National Center for Environmental Assessement. December.

U.S. EPA. 1997e. "Risk Assessment Issue Papers for: Carcinogenicity Information for Tetrachloroethylene (CASRN 127-18-4)." Superfund Technical Support Center. National Center for Environmental Assessement. December.

U.S. EPA. 1997f. "Risk Assessment Issue Papers for: Derivation of a Provisional Subchronic Inhalation RfC for Benzene (CASRN 71-43-2)." Superfund Technical Support Center. National Center for Environmental Assessement. December.

U.S. EPA. 1997g. *Mercury Study Report to Congress. Volume III: Fate and Transport of Mercury in the Environment.* Office of Air Quality Planning and Standards and Office of Research and Development. EPA-452/R-97-005. December.

U.S. EPA. 1997h. *Exposure Factors Handbook.* "Food Ingestion Factors". Volume II. EPA/600/P-95/002Fb. August.

U.S. EPA. 1998. *Screening Level Ecological Risk Assessment Protocol for Hazardous Waste Combustion Facilities.* Draft Interim Final. April.

Veith, G.D., K.J. Macek, S.R. Petrocelli, and J. Caroll. 1980. "An Evaluation of Using Partition Coefficients and Water Solubility to Estimate Bioconcentration Factors for Organic Chemicals in Fish." *Journal of Fish. Res. Board Can.* Prepublication Copy.

Verschueren, K. 1983. *Handbook of Environmental Data on Organic Chemicals.* Second Edition. Van Nostrand Reinhold Company. New York.

Weast, R.C. 1981. *Handbook of Chemistry and Physics.* 62nd Edition. Cleveland, Ohio. CRC Press.

Welsch-Pausch, K.M. McLachlan, and G. Umlauf. 1995. "Determination of the Principal Pathways of Polychlorinated Dibenzo-p-dioxins and Dibenzofurans to Lolium Multiflorum (Welsh Ray Grass)". *Environmental Science and Technology.* 29: 1090-1098.

U.S. EPA Region 6   U.S. EPA
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CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

(Page 1 of 4)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	154.21
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	368.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	4.93E-06 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.80E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.00E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.21E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.19E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	9.22E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	4.90E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.90E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.67E+02

CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

(Page 2 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.96E+02
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.48E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999975
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.69E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.48E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.98E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.98E-01

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for leafyaboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.66E+00
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.66E+00
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.32E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.31E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.80E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.32E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.83E-04
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.07E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

TABLE A-3-1

CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

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Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	6.00E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.10E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR ACETALDEHYDE (75-07-0)

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Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	44.05
T_m (K)	Montgomery and Welkom (1991)	--	149.6
Vp (atm)	--	--	ND
S (mg/L)	--	--	ND
H (atm·m^3/mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.72E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.33E-05
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	6.02E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.53E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.53E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.15E-02

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.81E-02
ksg (year)⁻¹	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0
Fv (unitless)	Fv value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.46E+00
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	6.78E+02
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.19E+01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.19E+01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	--	B-2-8	ND

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	--	B-3-8	ND
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.78E-09
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.51E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.83E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.78E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.19E-08
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.00E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1996d)	C-1-8	2.6E-03
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1996d)	C-1-7	7.7E-03
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	9.00E-03
Inhalation URF ($\mu g/m^3$)$^{-1}$	U.S. EPA (1997b)	C-2-1	2.20E-06
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	7.70E-03

TABLE A-3-2

CHEMICAL-SPECIFIC INPUTS FOR ACETALDEHYDE (75-07-0)

(Page 4 of 4)

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-3

CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	58.08
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	179.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.99E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	6.04E+05
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.88E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.87E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.15E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994g).	--	6.00E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.51E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.51E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.13E-02

TABLE A-3-3

CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.46E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	6.80E+02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.20E+01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegorund and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.20E+01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	$Bv_{leafy\ veg}$ value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for abovegorund produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.13E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.13E-03

TABLE A-3-3

CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.77E-09
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.51E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.82E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.77E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.19E-08
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	4.00E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	1.00E-01
$Oral\ CSF$ $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.50E-01
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR ACETONITRILE (75-05-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	41.05
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	318.1
Vp (atm)	Howard (1989-1993)	--	1.20E-01 at 25°C (solid)
S (mg/L)	Howard (1989-1993)	--	1.30E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.79E+01
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.14E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.40E-05
K_{ow} (unitless)	log K_{ow} value cited in Karickhoff and Long (1995).	--	4.57E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	7.69E-01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.69E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.76E-02

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The valus was then converted to a dry wight basis by using a moisture content of 87 percent.	B-2-10	6.43E+00
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	8.37E+02
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegrouns produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.09E+01
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegorund produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.09E+01
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.41E-10
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.41E-10

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.63E-09
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.15E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.39E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.63E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	9.06E-09
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.25E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	6.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.10E-02
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-5

CHEMICAL-SPECIFIC INPUTS FOR ACETOPHENONE (98-86-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	120.50
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	293.6
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	5.20E-04 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	6.10E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.03E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.73E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	4.37E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.69E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.69E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.02E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999999
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.06E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.92E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.37E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.37E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.04E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.04E-01

CHEMICAL-SPECIFIC INPUTS FOR ACETOPHENONE (98-86-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.47E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.10E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.33E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.47E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	8.66E-07
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.04E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-01
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from Oral RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.50E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-6

CHEMICAL-SPECIFIC INPUTS FOR ACROLEIN (107-02-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	56.06
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	185.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	3.50E-01 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	2.10E+05
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.34E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.92E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.22E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	9.80E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.39E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.39E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.05E-01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.54E+00
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.69E+02
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.92E+01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.92E+01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.86E-04
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.86E-04

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.78E-09
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.46E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.98E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.78E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.94E-08
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.80E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	2.0E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997)	C-2-3	2.0E-05
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR ACRYLONITRILE (107-13-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	53.06
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	189.6
Vp (atm)	Vp value cited in U.S. EPA (1995b) .	--	1.40E-01 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b) .	--	7.50E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.90E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.11E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.23E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.78E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.22E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.22E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.66E-01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.10E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.67E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.00E+02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.77E+01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.77E+01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.04E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.04E-03

TABLE A-3-7

CHEMICAL-SPECIFIC INPUTS FOR ACRYLONITRILE (107-13-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.41E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.47E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	5.41E-08
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.41E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.53E-08
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	4.80E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	1.0E-03
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	5.4E-01
RfC (mg/m³)	U.S. EPA (1997b)	C-2-3	2.0E-03
Inhalation URF (μg/m³)$^{-1}$	U.S. EPA (1997b)	C-2-1	6.8E-05
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	2.4E-01

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-8

CHEMICAL-SPECIFIC INPUTS FOR ALDRIN (309-00-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	364.93
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	377.1
Vp (atm)	Vp value cited in U.S. EPA (1992).	--	2.90E-11 at 25ºC (solid)
S (mg/L)	S value cited in U.S. EPA (1992).	--	7.84E-02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.35E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.43E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.40E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994f).	--	1.51E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	4.87E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.87E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction oF 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.65E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.95E+03

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	4.28E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.227325
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ wate}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.33E+04
$Br_{rootveg}$ $\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.73E+01
Br_{ag} $\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.04E-02
Br_{forage} $\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.04E-02
Bv_{ag} $\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.58E+06
Bv_{forage} $\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.58E+06

CHEMICAL-SPECIFIC INPUTS FOR ALDRIN (309-00-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.20E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.79E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.59E-02
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.20E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.99E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	BAFs were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. BCFs were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). FCMs were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.82E+05
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	3.00E-05
Oral CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997b)	C-1-7	1.70E+01
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.10E-04
Inhalation URF (μg/m^3)$^{-1}$	U.S.EPA (1997b)	C-2-1	4.90E-03
Inhalation CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997c)	C-2-2	1.70E+01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-9

CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	93.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	266.8
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	8.80E-04 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	3.60E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.28E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.56E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.01E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	9.55E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	8.23E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.23E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.17E-01
ksg (year)⁻¹	NC DEHNR (1996)	B-1-2; B-2-2; B-3-2; B-4-2	3.20E+01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999999
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.63E+00
$Br_{root \ veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	9.27E+01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with i that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.05E+01
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.05E+01
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-9	2.72E-01
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-9	2.72E-01

TABLE A-3-9

CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.59E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.40E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	2.90E-07
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.59E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	1.89E-07
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.27E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1996d)	C-1-8	2.9E-04
$Oral\ CSF$ $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	5.7E-03
RfC (mg/m³)	U.S. EPA (1997b)	C-2-3	1.0E-03
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	1.6E-03
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	5.7E-03

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	178.22
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	491.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	3.35E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	5.37E-02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.11E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.24E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.74E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	2.95E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.35E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.35E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.76E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	9.40E+02

CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	5.50E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999781
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.49E+02
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.76E+00
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.01E-01
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.01E-01
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.90E+01
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.90E+01

TABLE A-3-10

CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.34E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.41E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	8.98E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.34E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.85E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.60E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-01
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.1E+00
Inhalation URF (μg/m³)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-11

CHEMICAL-SPECIFIC INPUTS FOR ANTIMONY (7440-36-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	NA
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.73E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	8.96E-06
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	45 at pH=6.8
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	45 at pH=6.8
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	45 at pH=6.8
ksg (year)⁻¹	--	B-1-2; B-2-2; B-3-2; B-4-2	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000

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CHEMICAL-SPECIFIC INPUTS FOR ANTIMONY (7440-36-0)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}\right)$	--	B-2-10	ND
$Br_{rootveg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{rootveg}$.	B-2-10	3.00E-02
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	3.19E-02
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Bv values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{forage}.	B-3-8	2.00E-01
Br_{grain} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{grain} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{grain}.	B-3-8	2.00E-01
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	1.0E-04
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	1.0E-03

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
Ba_{pork} (day/kg FW)	--	B-3-12	ND
Ba_{egg} (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	4.00E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1995d)	C-1-8	4.0E-04
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.43E-03
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1016 (12674-11-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	257.9
T_m (K)	--	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	9.37E-07 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	5.71E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.23E-04
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.69E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	5.43E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.53E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.32E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.32E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.74E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	9.29E+02

CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1016 (12674-11-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	5.06E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999365
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.37E+03
$Br_{rootveg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.45E+01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.91E-02
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroudn produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.91E-02
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	7.52E+01
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	7.52E+01

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.01E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.37E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.71E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.01E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.03E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.33E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA(1997b)	C-1-8	7.00E-05
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.5E-04
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-13

CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1254 (11097-69-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	327.0
T_m (K)	Montgomery and Welkom (1991)	--	283.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.16E-07 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.00E-02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.79E-03
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.00E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.64E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.61E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.98E+05
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.83E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.37E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.93E+03

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	5.06E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.992833
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then ocnverted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.40E+04
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.42E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.00E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegorund produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.00E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.01E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.01E+01

TABLE A-3-13

CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1254 (11097-69-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.28E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.05E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.90E-02
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.28E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.19E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	6.66E+05
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-05
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	7.0E-05
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-14

CHEMICAL-SPECIFIC INPUTS FOR ARSENIC (7440-38-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	74.92
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	1,091 at 36 atm
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.07E-01
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.24E-05
K_{sw} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0
ksg (year)$^{-1}$	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	--	B-2-10	ND
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	8.00E-03
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value for fruits was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1993e) for garden fruits. Br_{ag} value for vegetables was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2×10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1993e). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	6.33E-03
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-8	3.60E-02
Br_{grain} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{grain} value was calculated by multiplying the uptake slope factors with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals.	B-3-8	4.00E-03
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

CHEMICAL-SPECIFIC INPUTS FOR ARSENIC (7440-38-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	6.0E-03
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	2.0E-03
Ba_{pork} (day/kg FW)	--	B-3-12	ND
Ba_{egg} (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4.)	B-4-26	2.00E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	3.0E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	1.5E+00
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.1E-03
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997b)	C-2-1	4.3E-03
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1996d)	C-2-2	1.5E+01

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR ATRAZINE (1912-24-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	215.68
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	444.1
Vp (atm)	Vp value cited in Budavari, O'Neil, Smith, and Heckelman (1989)	--	3.66×10^{-10} at 25°C (solid)
S (mg/L)	S value cited in Howard and others 1989 - 1993	--	3.00E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.63E-09
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.80E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.03E-06
K_{ow} (unitless)	log K_{ow} value cited in Karickhoff and Long (1995).	--	4.07E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.54E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.54E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.15E+01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.15E+00
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	1.04E+01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.944780
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture ocntent of 87 percent.	B-2-10	3.00E+01
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.96E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.20E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.20E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.28E+04
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.28E+04

CHEMICAL-SPECIFIC INPUTS FOR ATRAZINE (1912-24-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.23E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.02E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.24E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.23E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	8.07E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.67E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.5E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	2.2E-01
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.2E-01
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	6.3E-05
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	2.2E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR BARIUM (7440-39-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	137.33
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	983
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.14E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	8.26E-06
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
ksg (year)$^{-1}$	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000
	Biotransfer Factors for Plants		
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	--	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{root\ veg}$.	B-2-10	1.50E-02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	3.22E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Bv values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{forage}.	B-3-8	1.50E-01
Br_{grain} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{grain} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{grain}.	B-3-8	1.50E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

CHEMICAL-SPECIFIC INPUTS FOR BARIUM (7440-39-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	3.5E-04
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	1.5E-04
Ba_{pork} (day/kg FW)	—	B-3-12	ND
Ba_{egg} (day/kg FW)	—	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	—	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	—	B-4-26	NA
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	7.0E-02
$Oral\ CSF$ $(mg/kg/day)^{-1}$	—	C-1-7	ND
RfC (mg/m³)	U.S. EPA (1997b)	C-2-3	5.0E-04
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	—	C-2-1	ND
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	—	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-17

CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	329.6
Vp (atm)	Vp value cited in NC DEHNR (1997).	--	1.30E-03 at 25°C (solid)
S (mg/L)	S value cited in NC DEHNR (1997).	--	3.30E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.18E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.07E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.48E-06
K_{ow} (unitless)	K_{ow} value cited in NC DEHNR (1997).	--	3.00E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.01E-01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.01E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.51E+00

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CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.04E-01
ksg (year)$^{-1}$	Ksg value assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.50
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.72E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.42E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.42E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.00E-02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.00E-02

CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.38E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.54E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	9.12E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.38E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.95E-07
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	7.81E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.01E-01
Oral CSF (mg/kg/day)$^{-1}$		C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.50E-01
Inhalation URF (μg/m^3)$^{-1}$		C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$		C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	78.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	278.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.25E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.78E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.49E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.17E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.02E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	.137
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	--	6.20E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.65E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.48E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	3.89E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.66E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	2.67E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.25E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.25E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.92E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.92E-03

TABLE A-3-18

CHEMICAL-SPECIFIC INPUTS FOR BENZENE (71-43-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.09E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.44E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	4.17E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.09E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-14	2.72E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.48E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	Calculated from the RfC using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-1-8	1.70E-02
Oral CSF (mg/kg/day)⁻¹	U.S. EPA (1997b)	C-1-7	2.90E-02
RfC (mg/m³)	U.S.EPA (1997e)	C-2-3	6.00E-02
Inhalation URF (μg/m³)⁻¹	U.S. EPA (1997b)	C-2-1	8.30E-06
Inhalation CSF (mg/kg/day)⁻¹	U.S. EPA (1997c)	C-2-2	2.90E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-19

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)ANTHRACENE (56-55-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	228.28
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	433
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.03E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.28E-02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.62E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.47E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	6.21E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	4.77E+05
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	--	2.60E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.60E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.95E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.04E+04

TABLE A-3-19

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)ANTHRACENE (56-55-3)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.72E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.880520
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis using a moisture content of 87 percent.	B-2-10	5.48E+03
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	2.11E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.02E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.02E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi. (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi. (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.72E+04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi. (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.72E+04

TABLE A-3-19

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)ANTHRACENE (56-55-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.79E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.20E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	1.45E-02
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.79E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	9.46E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.10E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	calculated by multiplying the Oral CSF for Benzo(a)pyrene by the relative potency factor for Benzo(a)anthracene of 0.1 (U.S.EPA 1993e)	C-1-7	7.31E-01
RfC (mg/m³)	--	C-2-3	ND
Inhalation URF ($\mu g/m^3$)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	2.10E-04
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	7.31E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-20

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	252.3
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	452
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	6.43E-12 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.94E-03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.36E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.18E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database in U.S. EPA (1994d).	B-4-20	5.85E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.35E+06
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	--	9.69E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.69E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.27E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25; B-2-10	3.87E+04

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	4.77E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.264620
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.22E+04
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see Section A3.4.2 of Appendix A-3).	B-2-10	1.26E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.11E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.11E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.25E+05
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.25E+05

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.07E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.38E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 in Appendix A-3).	B-3-12	4.10E-02
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.07E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 in Appendix A-3).	B-3-14	2.67E-02
BCF_{fish} (L/kg, FW tissue)	—	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	9.95E+03
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	—	C-1-8	ND
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	7.30E+00
RfC (mg/m^3)	—	C-2-3	ND
$Inhalation\ URF$ (μg/m^3)$^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	2.10E-03
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	7.30E+00

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	--	252.32
T_m (K)	Montgomery and Welkom (1991)	--	441
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	1.06E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	4.33E-03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.18E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.28E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	5.49E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.59E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	8.36E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.36E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.27E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.34E+04

CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.15E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.821980
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.39E+04
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.66E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.007E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.007E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.65E+04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.65E+04

CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.27E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.00E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.84E-02
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.27E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.16E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	9.95E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	Calculated by multiplying the Oral CSF for Benzo(a)pyrene by the relative potency factor for Benzo(b)fluoranthene of 0.1 (U.S.EPA 1993e).	C-1-7	7.3E-01
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	2.1E-01
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	7.3E-01

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	252.32
T_m (K)	Montgomery and Welkom (1991)	--	490
Vp (atm)	U.S. EPA (1994b)	--	1.32E-12 at 25°C (solid)
S (mg/L)	U.S. EPA (1994b)	--	8.0E-04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.15E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.28E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	5.49E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	1.56E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	8.32E-05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.32E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.24E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.33E+04

CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Lyman, Reehl, and Rosenblatt (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.18E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.148943
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.38E+04
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.66E+00
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.01E-02
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.01E-02
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.40E+05
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.40E+05

CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.26E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.98E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.82E-02
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.26E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.14E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	9.95E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	Calculated by multiplying the Oral CSF for Benzo(a)pyrene by the relative potency factor for benzo(k)fluoranthene of 0.01 (U.S.EPA 1993?)	C-1-7	7.3E-02
RfC (mg/m³)	--	C-2-3	ND
Inhalation URF (μg/m³)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	2.1E-05
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	7.3E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-23

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

(Page 1 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	122.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	395.5
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	8.57E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.15E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.22E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.36E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.80E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	7.60E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH K_{oc} 1 31.98 2 31.80 3 30.13 4 19.81 5 4.81 6 0.99 7 0.55 8 0.50 9 0.50 10 0.50 11 0.50 12 0.50 13 0.50 14 0.50
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.50E-03

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

(Page 2 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.13E-02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.20E-02
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	1.26E+02
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999992
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \; DW \; plant}{\mu g/mL \; soil \; water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.28E+01
$Br_{root\,veg}$ $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{root\,veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.33E+03
Br_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.17E+00
Br_{forage} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.17E+00
Bv_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.69E+01

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

(Page 3 of 4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} ($\frac{\mu g/g \; DW \; plant}{\mu g/g \; air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.69E+01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.04E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.91E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.31E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.04E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.51E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.58E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	4.00E+00
$Oral \; CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.40E+01

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

(Page 4 of 4)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks (continued)			
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-24

CHEMICAL-SPECIFIC INPUTS FOR BENZONITRILE (100-47-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	103.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	285.85
Vp (atm)	--	--	ND
S (mg/L)	--	--	ND
H (atm·m³/mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.45E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.43E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	3.63E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.33E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.33E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.75E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	9.33E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.00E+01
$Br_{root\,veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root\,veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.29E+00
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.86E+00
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.86E+00
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	--	B-2-8	ND
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	--	B-3-8	ND

CHEMICAL-SPECIFIC INPUTS FOR BENZONITRILE (100-47-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.88E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	9.12E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.10E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.88E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	7.20E-07
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	9.03E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-25

CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	108.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	288.29
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.40E-04 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1992a).	--	4.00E+04
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.78E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.89E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.38E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	--	1.26E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.02E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.02E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.66E-01

CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.09E-01
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999996
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.94E+00
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	7.77E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.95E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.95E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.19E+00
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.19E+00

CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.00E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.16E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.83E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.00E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.5E-07
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.04E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.00E-01
Oral CSF (mg/kg/day)$^{-1}$		C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.10
Inhalation URF (μg/m^3)$^{-1}$		C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$		C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	126.58
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	225.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	1.60E-03 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	4.90E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.13E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.43E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.80E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	2.30E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.71E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.71E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.03E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.08E-01

TABLE A-3-26

CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.09E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.75E+00
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.49E+02
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.39E+01
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.39E+01
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.28E-04
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.28E-04

TABLE A-3-26

CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.83E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.78E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	6.99E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.83E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.56E-08
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.11E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	1.70E-01
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	4.90E-05
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	1.70E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-27

CHEMICAL-SPECIFIC INPUTS FOR BERYLLIUM (7440-41-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	9.01
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	1,560
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.39E-01
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	5.08E-05
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0
ksg (year)⁻¹	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
F_v (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000
Biotransfer Factors for Plants			
RCF $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water} \right)$	--	B-2-10	ND
$Br_{rootveg}$ $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil} \right)$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{rootveg}$.	B-2-10	1.50E-03
Br_{ag} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil} \right)$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	2.58E-03
Br_{forage} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil} \right)$	Br_{forage} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Bv values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{forage}.	B-3-8	1.00E-02
Br_{grain} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil} \right)$	Br_{grain} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{grain}.	B-3-8	1.50E-03
Bv_{ag} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	9.0E-07
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	1.0E-03
Ba_{pork} (day/kg FW)	--	B-3-12	ND
Ba_{egg} (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	4.20E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.00E-03
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	4.3E+00
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	2.0E-02
Inhalation URF (μg/m^3)$^{-1}$	U.S. EPA (1997b)	C-2-1	2.4E-03
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	8.4E+00

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-28

CHEMICAL-SPECIFIC INPUTS FOR ALPHA-BHC (319-84-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	290.0
T_m (K)	Montgomery and Welkom (1991)	--	432.2
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	5.61E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.40E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.78E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	0.0191
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.04E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994g).	--	6.30E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.76E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.76E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.32E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	7.05E+01

TABLE A-3-28

CHEMICAL-SPECIFIC INPUTS FOR ALPHA-BHC (319-84-6)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.87E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999500
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was hen converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.02E+02
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.15E+01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.47E-01
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.47E-01
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	9.17E+01
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	9.17E+01

CHEMICAL-SPECIFIC INPUTS FOR ALPHA-BHC (319-84-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.00E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.58E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.92E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.00E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.25E-04
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)(see Appendix A-3).	B-4-26	4.54E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997b)	C-1-7	6.30E+00
RfC (mg/m³)	--	C-2-3	ND
Inhalation URF (μg/m³)$^{-1}$	U.S.EPA (1997b)	C-2-1	1.80E-03
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	6.3E+00

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-29

CHEMICAL-SPECIFIC INPUTS FOR BETA-BHC (319-85-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	290.83
T_m (K)	Montgomery and Welkom (1991)	--	582.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	6.45E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	5.42E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.46E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.9E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.40E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994g).	--	6.81E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.14E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.14E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.60E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.56E+01

CHEMICAL-SPECIFIC INPUTS FOR BETA-BHC (319-85-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.04E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.998571
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.14E+02
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.00E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{leafy\ veg}$ value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.36E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.36E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.95E+03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.95E+03

TABLE A-3-29

CHEMICAL-SPECIFIC INPUTS FOR BETA-BHC (319-85-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.41E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.71E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.07E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.41E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.35E-04
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were obtained from U.S. EPA (1995b). BCF_{fish} value cited in U.S. EPA (1995b).	B-4-26	4.82E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S.EPA(1997c)	C-1-7	1.80E+00
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	U.S.EPA (1997b)	C-2-1	1.80E-03
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	1.8E+00

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-30

CHEMICAL-SPECIFIC INPUTS FOR BIS(2-CHLORETHYL)ETHER (111-44-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	143.02
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	223.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	1.76E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.18E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.13E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.40E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.70E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	2.00E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	7.60E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.60E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.70E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.04E+00
ksg (year)⁻¹	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.64E+00
$Br_{root\,veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\,veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.14E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.85E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.85E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.37E-02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.37E-02

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.59E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.02E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	6.08E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.59E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.97E-07
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.74E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	1.1E+00
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	U.S. EPA (1997e)	C-2-1	3.3E-04
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	1.1E+00

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	163.83
T_m (K)	Montgomery and Welkom (1991)	--	218.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	7.68E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.97E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.17E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.98E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.06E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.06E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.38E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.38E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.03E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.15E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.47E+01
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.74E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.61E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.61E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.53E-03
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.53E-03

CHEMICAL-SPECIFIC INPUTS FOR BROMODICHLOROMETHANE (75-27-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	8.42E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.66E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	3.22E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	8.42E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	2.10E-06
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.04E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.00E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	6.20E-02
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	7.00E-02
$Inhalation\ URF$ (μg/m³)$^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	1.80E-05
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	6.20E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR BROMOFORM (75-25-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	252.77
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	280.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	7.82E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.21E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.16E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.41E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.03E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.24E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.26E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.26E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.45E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.04E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water} \right)$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.13E+01
$Br_{root \ veg}$ $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil} \right)$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.69E+01
Br_{ag} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil} \right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.70E+00
Br_{forage} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil} \right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.70E+00
Bv_{ag} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air} \right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.89E-02
Bv_{forage} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air} \right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.89E-02

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.78E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.63E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	6.81E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.78E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	4.44E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.60E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.00E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	7.90E-03
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.00E-02
$Inhalation\ URF$ (μg/m^3)$^{-1}$	U.S. EPA (1997b)	C-2-1	1.10E-06
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	3.90E-03

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	249.2
T_m (K)	Montgomery and Welkom (1991)	--	291.8
Vp (atm)	Vp value cited in Montgomery and Welkom (1991).	--	1.97E-06 at 25°C (liquid)
S (mg/L)	--	--	ND
H (atm·m³/mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.98E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.83E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.10E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.21E+05
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.21E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.09E+03

TABLE A-3-33

CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.85E+03
ksg (year)⁻¹	Ksg value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999699
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.78E+03
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.47E+00
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.72E-02
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.72E-02
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	--	B-2-8	ND
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	--	B-3-8	ND

CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	8.74E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.76E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.34E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	8.74E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.18E-03
BCF_{fish} (unitless FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.46E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	5.80E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.03E-01
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-34

CHEMICAL-SPECIFIC INPUTS FOR BUTYLBENZYLPHTHALATE (85-68-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	--	312.39
T_m (K)	Howard (1989-1993)	--	238.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.58E-08 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.58E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.91E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.65E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.17E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.59E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.37E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.37E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.03E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.50E+02
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.963708

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Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\cdot\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}\cdot$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	5.87E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.27E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.09E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.09E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.46E+03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.46E+03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.06E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.50E-04

CHEMICAL-SPECIFIC INPUTS FOR BUTYLBENZYLPHTHALATE (85-68-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.87E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.06E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.13E-04
BCF_{fish} (L/kg FW tissue)	---	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.35E+03
$BSAF_{fish}$ (unitless)	---	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.00E-01
$Oral\ CSF$ (mg/kg/day)$^{-1}$	---	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.00E-01
$Inhalation\ URF$ (μg/m^3)$^{-1}$	---	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	---	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-35

CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

(Page 1 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	112.41
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	594.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.16E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	9.45E-06
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0
ksg (year)⁻¹	--	B-1-2; B-2-2; B-3-2; B-4-2	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}\right)$	--	B-2-10	ND
$Br_{rootveg}$ $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil}\right)$	$Br_{rootveg}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	6.40E-02
Br_{ag} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil}\right)$	Br_{ag} value for fruits was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1993e) for garden fruits. Br_{ag} value for vegetables was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2×10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1993e). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	1.25E-01
Br_{forage} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil}\right)$	Br_{forage} value was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-8	3.64E-01
Br_{grain} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil}\right)$	Br_{grain} value was calculated by multiplying the uptake slope factors with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals.	B-3-8	6.20E-02
Bv_{ag} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air}\right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air}\right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

(Page 3 of 4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 87% moisture content in milk.	B-3-11	6.50E-06
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in beef.	B-3-10	1.20E-04
Ba_{pork} (day/kg FW)	Ba_{pork} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 4.7 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in pork.	B-3-12	1.91E-04
Ba_{egg} (day/kg FW)	Ba_{egg} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in eggs.	B-3-13	2.50E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in chicken.	B-3-14	1.06E-01
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	2.50E+02
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD *(water)* (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-04
RfD *(food)* (mg/kg/day)	U.S. EPA (1997b)		1.0E-03
Oral CSF (mg/kg/day)$^{-1}$	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-1-7	6.3E+00
RfC (mg/m³)	Calculated from RfD *(food)* value using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	3.5E-03
Inhalation URF (μg/m³)$^{-1}$	U.S. EPA (1997b)	C-2-1	1.8E-03
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	6.3E+00

CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

(Page 4 of 4)

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR CARBON DISULFIDE (75-15-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	76.14
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	161.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	4.47E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.67E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.27E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.04E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.29E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.00E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.14E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.14E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.86E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.06E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.44E+01
$Br_{root\ veg}$ $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.79E+01
Br_{ag} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.70E+00
Br_{forage} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.70E+00
Bv_{ag} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.92E-04
Bv_{forage} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.92E-04

TABLE A-3-36

CHEMICAL-SPECIFIC INPUTS FOR CARBON DISULFIDE (75-15-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.94E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.51E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	3.04E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.94E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	1.98E-06
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.95E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-01
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	7.00E-01
$Inhalation\ URF$ ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR CARBON TETRACHLORIDE (56-23-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	153.84
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	250.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.48E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.92E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.87E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.56E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.77E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.21E+02
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	--	1.52E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.52E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.14E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.08E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.50E+01
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.30E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.04E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.04E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.52E-03
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.52E-03

CHEMICAL-SPECIFIC INPUTS FOR CARBON TETRACHLORIDE (56-23-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.14E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.30E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.58E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.14E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	1.03E-05
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	3.00E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	7.00E-04
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	1.30E-01
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.50E-03
Inhalation URF (μg/m^3)$^{-1}$	U.S. EPA (1997b)	C-2-1	1.50E-05
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	5.30E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR CHLORDANE (57-74-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	409.80
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	381.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	3.55E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	5.51E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.64E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.18E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.37E-06
K_{sw} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	8.66E+05
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	--	5.13E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.13E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.85E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.05E+03
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.83E-01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.997476
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.67E+03
$Br_{root \ veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	1.69E+01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.43E-02
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.43E-02
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.46E+03
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.46E+03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.88E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.17E-02

CHEMICAL-SPECIFIC INPUTS FOR CHLORDANE (57-74-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	2.63E-02
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.88E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	1.72E-02
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.07E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-01
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	3.50E-01
RfC (mg/m^3)	U.S.EPA (1997b)	C-2-3	7.00E-04
$Inhalation\ URF$ (µg/m^3)$^{-1}$	U.S. EPA (1997b)	C-2-1	1.00E-04
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	3.50E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR CHLORINE (7782-50-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	71.90
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	172.1
Vp (atm)	--	--	ND
S (mg/L)	--	--	ND
H (atm·m³/mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm²/s)	--	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.10E-01
D_w (cm²/s)	--	B-4-20	1.27E-05
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	--	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	ND
Kd_{sw} (L/Kg)	--	B-4-16; B-4-18; B-4-24	ND
Kd_{bs} (mL/g)	--	B-4-16; B-4-25	ND
ksg (year)⁻¹	--	B-1-2; B-2-2; B-3-2; B-4-2	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\left(\frac{\mu g/g\ WW\ plant}{\mu g/mL\ soil\ water}\right)$	--	B-2-10	ND
$Br_{rootveg}$ $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	--	B-2-10	ND
Br_{ag} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	--	B-2-9	ND
Br_{forage} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	--	B-3-9	ND
Bv_{ag} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	--	B-2-8	NA
Bv_{forage} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	--	B-3-8	NA
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all inorganics, except cadmium, mercury, selenium, and zinc.	B-3-11	1.50E-02
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all inorganics, except cadmium, mercury, selenium, and zinc.	B-3-10	8.00E-02
Ba_{pork} (day/kg FW)	--	B-3-12	ND
BCF_{egg} (day/kg FW)	--	B-3-13	ND
BCF_{chick} (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW)	--	B-4-26	ND
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

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CHEMICAL-SPECIFIC INPUTS FOR CHLORINE (7782-50-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA 1994e or U.S. EPA 1995c	C-1-8	1.0E-01
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.5E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	142.58
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	328.6
Vp (atm)	--	--	ND
S (mg/L)	U.S.EPA (1992a)	--	3.85E+03
H (atm·m³/mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.96E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	8.06E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.26E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.71E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.71E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.78E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.48E+02

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Lucius (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.10E+01
Fv (unitless)	--	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	ND
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	6.30E+01
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.70E+00
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.25E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.25E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	--	B-2-8	ND
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	--	B-3-8	ND

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.00E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.16E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.83E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.00E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.50E-05
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.34E+02
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	—	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	—	C-1-7	ND
RfC (mg/m³)	—	C-2-3	ND
Inhalation URF (μg/m³)$^{-1}$	—	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	—	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR P-CHLOROANILINE (106-47-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	127.57
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	345.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	3.09E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.36E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.17E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.80E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.02E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	7.40E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	K_{oc} is 41 for pH range of 4.9 to 8
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.06E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.05E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.63E+00

CHEMICAL-SPECIFIC INPUTS FOR P-CHLOROANILINE (106-47-8)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due a a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999993
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.27E+01
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.12E+01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.22E+00
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.22E+00
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.66E+00
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.66E+00

CHEMICAL-SPECIFIC INPUTS FOR P-CHLOROANILINE (106-47-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.88E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.86E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.25E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.88E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.47E-06
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.55E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	4.00E-03
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.40E-02
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-42

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	112.56
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	228.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.59E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	4.09E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.38E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.35E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.49E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	6.16E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.24E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.24E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.68E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.96E+00
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.69E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	1.000000

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \; DW \; plant}{\mu g/mL \; soil \; water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.90E+01
$Br_{root \; veg}$ $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{root \; veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.74E+01
Br_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	9.45E-01
Br_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	9.45E-01
Bv_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.19E-02
Bv_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.19E-02
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.89E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.55E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.87E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.89E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.22E-05

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	7.76E+01
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-02
Oral CSF (mg/kg/day)$^{-1}$	—	C-1-7	ND
RfC (mg/m³)	U.S. EPA (1997c)	C-2-3	2.0E-02
Inhalation URF (μg/m³)$^{-1}$	—	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	—	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	325.20
T_m (K)	Howard (1989-1993)	--	309.0
Vp (atm)	Howard (1989-1993)	--	2.90E-09 at 25°C (solid)
S (mg/L)	Howard (1989-1993)	--	1.30E+01
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.24E-08
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.65E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	4.72E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	2.40E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.69E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.69E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.77E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.48E+02

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.23E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.861816
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	5.54E+02
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.50E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.14E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.14E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.57E+04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.57E+04

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.91E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.03E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.29E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.91E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.76E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.03E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-02
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1995b)	C-1-7	2.7E-01
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E-02
Inhalation URF (μg/m^3)$^{-1}$	U.S. EPA (1997c)	C-2-1	7.8E-06
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	2.7E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-44

CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

(Page 1 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Howard 1989-1993	--	86.47
T_m (K)	Howard 1989-1993	--	126.6
Vp (atm)	Vp value cited in Howard 1989-1993.	--	5.63 at 25°C (liquid)
S (mg/L)	Howard 1989-1993	--	2.90E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.68E-01
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.72E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.13E-05
K_{ow} (unitless)	Calculated using the log K_{ow} value cited in Howard 1989-1993.	--	1.20E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.83E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.83E-02

CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

(Page 2 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.93E-01
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) OR Howard (1989-1993) OR Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.88E+00
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	8.01E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	9.21E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	9.21E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.69E-06

TABLE A-3-44

CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

(Page 3 of 4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (continued)			
Bv_{forage} ($\frac{\mu g/g \ DW \ plant}{\mu g/g \ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.69E-06
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.53E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.01E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.65E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.53E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.38E-07
BCF_{fish} (L/kg, FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.89E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	Calculated from RfC using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-1-8	1.40E+01
Oral CSF (mg/kg/day)⁻¹		C-1-7	ND
RfC (mg/m³)	U.S. EPA (1997b)	C-2-3	5.00+01
Inhalation URF ($\mu g/m^3$)⁻¹		C-2-1	ND
Inhalation CSF (mg/kg/day)⁻¹		C-2-2	ND

TABLE A-3-44

CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

(Page 4 of 4)

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-45

CHEMICAL-SPECIFIC INPUTS FOR CHLOROETHANE (75-00-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	64.52
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	441.8
Vp (atm)	Vp value cited in Lucius et al. (1992).	--	159.88 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1994a)	--	5.74E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.80
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.27E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.53E-06
K_{ow} (unitless)	K_{ow} value calculated from log K_{ow} value cited in U.S. EPA (1995a).	--	1.26E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.71E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.71E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.78E+01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.48E+01
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	6.72E+02
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then ocnverted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.30E+01
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.70E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.25E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.25E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.05E-05
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.05E-05

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.00E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.16E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.83E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.00E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.50E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.34E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997a)	C-1-8	4.00E-01
Oral CSF (mg/kg/day)$^{-1}$		C-1-7	ND
RfC (mg/m³)	U.S. EPA (1997b)	C-2-3	1.00E+01
Inhalation URF (μg/m³)$^{-1}$		C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$		C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (67-66-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	119.39
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	209.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.69E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.96E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.03E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.17E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.09E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	8.90E+01
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	--	5.30E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.98E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.12E+00

CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (67-66-3)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.37E+01
$Br_{rootveg}$ $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil}\right)$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	2.58E+01
Br_{ag} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.89E+00
Br_{forage} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.89E+00
Bv_{ag} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.65E-03
Bv_{forage} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.65E-03

CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (67-66-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.07E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.23E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	2.71E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.07E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	1.76E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	3.59E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-02
$Oral\ CSF$ $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	6.10E-03
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.50E-02
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	U.S. EPA (1997b)	C-2-1	2.30E-05
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-2-2	8.10E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-47

CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER (39638-32-9)

(Page 1 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	171.07
T_m (K)	Montgomery and Welkom (1991)	--	369.9
Vp (atm)	Montgomery and Welkom (1991)	--	7.00E-03 at 25°C (solid)
S (mg/L)	Montgomery and Welkom (1991)	--	1.70E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.04E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.61E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.38E-06
K_{ow} (unitless)	K_{ow} value cited in Howard (1989 - 1993).	--	3.80E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.46E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.46E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.46E-02

**CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER
(39638-32-9)**

(Page 2 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.82E+00
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.88E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.98E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.25E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-9	4.44-02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.44E-02

CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER
(39638-32-9)

(Page 3 of 4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.02E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	9.55E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.16E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.02E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	7.54E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.38E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

TABLE A-3-47

CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER (39638-32-9)

(Page 4 of 4)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	4.0E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.4E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	162.61
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	332.6
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	1.05E-05 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	1.20E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.43E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.64E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.24E-06
K_{ow} (unitless)	Montgomery and Welkom (1991)	--	1.17E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	7.14E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.14E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.36E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.86E+02

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999974
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.23E+02
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-9; B-2-10; B-3-9	4.51E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.72E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-10	1.72E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-9	8.46E+00
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-9	8.46E+00

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.33E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.95E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.57E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.33E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.33E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	9.60E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	8.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	2.80E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	128.56
T_m (K)	Montgomery and Welkom (1991)	--	282.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.77E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.15E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.66E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.01E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.46E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.45E+02
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH K_{oc} 1 398.0 2 398.0 3 398.0 4 398.0 5 397.9 6 396.9 7 387.3 8 311.8 9 108.7 10 19.43 11 7.39 12 6.14 13 6.01 14 6.00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.87E+00

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	2.90E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	1.55E+01
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $$\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.70E+01
$Br_{rootveg}$ $$(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-9; B-2-10; B-3-9	4.40E+00
Br_{ag} $$(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.18E+00
Br_{forage} $$(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-10	2.18E+00
Bv_{ag} $$(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-9	6.76E-01

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} ($\frac{\mu g/g \ DW \ plant}{\mu g/g \ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.76E-01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.15E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.64E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.41E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.15E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.88E-06
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.59E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-03
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.80E-02
Inhalation URF ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-50

CHEMICAL-SPECIFIC INPUTS FOR 3-CHLOROPHENYL-PHENYLETHER (7005-72-3)

(Page 1 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	204.66
T_m (K)	Montgomery and Welkom (1991)	--	265.1
Vp (atm)	Vp value cited in Montgomery and Welkom (1991).	--	3.55E-06 at 25°C (liquid)
S (mg/L)	S value cited in Montgomery and Welkom (1991).	--	3.30E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.20E-04
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.82E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.42E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	5.85E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	7.40E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.40E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.55E+03

CHEMICAL-SPECIFIC INPUTS FOR 3-CHLOROPHENYL-PHENYLETHER
(7005-72-3)

(Page 2 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.96E+03
ksg (year)⁻¹	Ksg value was assumed to be zero due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999832
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.09E+03
$Br_{rootveg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.48E+00
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.80E-02
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.80E-02
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.03E+01

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.03E+01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.65E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.47E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.78E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.65E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.16E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	6.06E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	--	C-2-3	ND
Inhalation URF ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

TABLE A-3-50

CHEMICAL-SPECIFIC INPUTS FOR 3-CHLOROPHENYL-PHENYLETHER
(7005-72-3)

(Page 4 of 4)

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-51

CHEMICAL-SPECIFIC INPUTS FOR CHLOROPYRIFOS (2921-88-2)

(Page 1 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	350.59
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	314.6
Vp (atm)	Vp value cited in Howard (1989-1993).	--	1.32E-03 at 25°C (solid)
S (mg/L)	S value cited in Howard (1989-1993).	--	5.00E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.26E-02
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.82E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.42E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	1.82E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.79E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.79E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.35E+03

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	7.18E+02
ksg (year)⁻¹	Ksg value was assumed to 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.61E+03
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.46E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.53E-02
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.53E-02
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for abovegorund produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.42E-01

CHEMICAL-SPECIFIC INPUTS FOR CHLOROPYRIFOS (2921-88-2)

(Page 3 of 4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (continued)			
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.42E-01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.45E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.57E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	5.53E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.45E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.61E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.81E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

CHEMICAL-SPECIFIC INPUTS FOR CHLOROPYRIFOS (2921-88-2)

(Page 4 of 4)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.03E-03
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E-02
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (7440-47-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	52
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	2,173.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.01E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	B-4-20	4.63E-05
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	--	B-1-2; B-2-2; B-3-2; B-4-2	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	--	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{rootveg}$.	B-2-10	4.50E-03
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	4.88E-03
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Bv values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{forage}.	B-3-8	7.50E-03
Br_{grain} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{grain} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{grain}.	B-3-8	4.50E-03
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} ($\frac{\mu g/g \ DW \ plant}{\mu g/g \ air}$)	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	1.5E-03
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	5.5E-03
Ba_{pork} (day/kg FW)		B-3-12	ND
Ba_{egg} (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from Thompson, Burton, Quinn, and Ng (1972) for freshwater and marine fish.	B-4-26	2.83E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	RfD value cited in U.S. EPA (1995c) for Chromium (III).	C-1-8	1.0E+00
Oral CSF (mg/kg/day)[-1]	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	3.5E+00
Inhalation URF ($\mu g/m^3$)[-1]	--	C-2-1	ND
Inhalation CSF (mg/kg/day)[-1]	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR HEXAVALENT CHROMIUM (18540-29-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	52
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	2,173.0
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.36E-01
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.58E-05
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
ksg (year)$^{-1}$	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

CHEMICAL-SPECIFIC INPUTS FOR HEXAVALENT CHROMIUM (18540-29-9)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \; DW \; plant}{\mu g/mL \; soil \; water}$	—	B-2-10	ND
$Br_{root\,veg}$ $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{root\,veg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{root\,veg}$.	B-2-10	4.50E-03
Br_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	4.88E-03
Br_{forage} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Bv values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{forage}.	B-3-8	7.50E-03
Br_{grain} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{grain} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{grain}.	B-3-8	4.50E-03
Bv_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

CHEMICAL-SPECIFIC INPUTS FOR HEXAVALENT CHROMIUM (18540-29-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	1.5E-03
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	5.5E-03
Ba_{pork} (day/kg FW)	--	B-3-12	ND
Ba_{egg} (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	BCF values were obtained from U.S. EPA (1995b) for all metals, except lead and mercury.	B-4-26	3.0E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	RfD value cited in U.S. EPA (1997b) for Chromium (VI).	C-1-8	5.0E-03
Oral CSF $(mg/kg/day)^{-1}$	Calculated based on *Inhalation URF* using inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-1-7	4.1E+01
RfC (mg/m³)	Calculated from *RfD* using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.8E-02
Inhalation URF $(\mu g/m^3)^{-1}$	*Inhalation URF* value cited in U.S. EPA (1997b) for Chromium (VI).	C-2-1	1.2E-02
Inhalation CSF $(mg/kg/day)^{-1}$	*Inhalation CSF* value cited in U.S. EPA (1997c) for Chromium (VI).	C-2-2	4.1E+01

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-54

CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	228.28
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	527.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.03E-11 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.94E-03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.21E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.48E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	6.21E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.48E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.97E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.97E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.23E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.19E+04

CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.53E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.761276
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.10E+03
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.05E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.866E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.866E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.97E+04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.97E+04

CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.355E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.377E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.67E-02
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.35E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.09E-02
BCF_{fish} (L/kg FW tissue)	—	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	6.03E+03
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	—	C-1-8	ND
$Oral\ CSF$ (mg/kg/day)$^{-1}$	Calculated by multiplying the $Oral\ CSF$ for Benzo(a)pyrene by the relative potency factor for chrysene of 0.001 (U.S.EPA 1993e)	C-1-7	7.3E-03
RfC (mg/m³)	—	C-2-3	ND
$Inhalation\ URF$ ($\mu g/m^3$)$^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	2.1E-06
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	108.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	284.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	1.90E-04 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	2.30E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.93E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.93E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.30E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	--	9.10E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.78E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.78E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.58E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.91E+00

TABLE A-3-55

CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	8.72E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999997
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.38E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.89E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.86E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.86E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	7.64E+00
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	7.64E+00

CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.23E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.29E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.77E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.23E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.86E-06
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.81E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.8E+00
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-56

CHEMICAL-SPECIFIC INPUTS FOR O-CRESOL (95-48-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	108.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	303.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	4.16E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.77E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.62E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.88E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.41E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.05E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.34E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.34E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.0E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.14E+00

CHEMICAL-SPECIFIC INPUTS FOR O-CRESOL (95-48-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999999
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.47E+01
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.75E+01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.63E+00
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.63E+00
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.89E+00
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.89E+00

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	8.34E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.64E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.19E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	8.34E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.08E-06
BCF_{fish} (L/kg, FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.02E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.80E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	108.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	308.6
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	1.70E-04 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	2.30E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.99E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.93E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.30E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	--	8.70E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.61E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.61E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.46E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.84E+00

CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.79E+02
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999997
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.35E+01
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.94E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.93E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.93E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	8.13E+00
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	8.13E+00

TABLE A-3-57

CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.91E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.19E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.65E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.91E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.73E-06
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.75E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	5.00E-03
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.80E-02
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-58

CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	120.19
T_m (K)	U.S. EPA (1995b)	--	177
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	6.00E-03 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	5.60E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.29E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.50E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.83E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	--	4.10E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.31E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.31E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.98E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.72E+02

CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.16E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999998
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.47E+02
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.58E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.16E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.16E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.06E-02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.06E-02

CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.26E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.03E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.25E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.26E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	8.13E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.28E+02
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-01
$Oral\ CSF$ (mg/kg/day)$^{-1}$	—	C-1-7	NA
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	4.00E-01
$Inhalation\ URF$ (μg/m^3)$^{-1}$	—	C-2-1	NA
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	—	C-2-2	NA

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S.EPA (1992a)	--	26.017
T_m (K)	--	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.82E-02 at 25°C (solid)
S (mg/L)	--	--	ND
H (atm·m³/mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.48E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	2.10E-05
K_{ow} (unitless)	--	--	ND
K_{oc} (mL/g)	--	--	ND
Kd_s (cm³/g)	--	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	ND
Kd_{sw} (L/Kg)	--	B-4-16; B-4-18; B-4-24	ND
Kd_{bs} (cm³/g)	--	B-4-16; B-4-25	ND
ksg (year)$^{-1}$	Ksg value was assumed to be zero due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	—	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	—	B-2-10	ND
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	—	B-2-9	ND
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	—	B-3-9	ND
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	—	B-2-8	ND
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	—	B-3-8	ND
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	—	B-3-11	ND
Ba_{beef} (day/kg FW)	—	B-3-10	ND
Ba_{pork} (day/kg FW)	—	B-3-12	ND
Ba_{eggs} (day/kg FW)	—	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	—	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—see Appendix A-3.	B-4-26	6.33E+02
BAF_{fish} (L/kg FW)	—	B-4-27	ND

CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks (Continued)			
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E-02
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDD (72-54-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	320.05
T_m (K)	Montgomery and Welkom (1991)	--	380.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.14E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.33E-02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.98E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.69E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.76E-06
K_{sw} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.32E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	4.58E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.58E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.44E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.83E+03

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.34E-02
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.925394
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.20E+04
$Br_{rootveg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.62E+01
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.12E-02
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.12E-02
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.70E+04
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.70E+04

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDD (72-54-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.05E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.31E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.01E-02
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.05E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.62E-02
BCF_{fish} (L/kg, FW tissue)	—	B-4-26	NA
BAF_{fish} (L/kg FW)	BAFs were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. BCFs were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). FCMs were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.25E+05
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	—	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997b)	C-1-7	2.40E-01
RfC (mg/m^3)	—	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	6.90E-05
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	2.40E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	--	319.03
T_m (K)	Montgomery and Welkom (1991)	--	361.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	7.45E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.92E-02
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.24E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.78E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.80E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	8.64E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.64E+06
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.48E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.46E+03

TABLE A-3-61

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.34E-02
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.981338
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.53E+04
$Br_{rootveg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.77E+01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroun produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	9.37E-03
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	9.37E-03
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.08E+03
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.08E+03

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.43E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.53E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	5.49E-02
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.43E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.58E-02
BCF_{fish} (L/kg, FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.53E+05
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997b)	C-1-7	3.40E-01
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from the Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	9.7E-05
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	3.40E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDT (50-29-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	354.49
T_m (K)	Montgomery and Welkom (1991)	--	381.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	5.17E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.41E-03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.37E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.48E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.48E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.17E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	6.78E+05
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.78E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.08E+04
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.71E+04

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.34E-02
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.851957
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.10E+04
$Br_{rootveg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.62E+00
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.20E-02
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.20E-02
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for above ground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.03E+03
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.03E+03

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDT (50-29-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.33E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.95E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.57E-02
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.33E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.33E-02
BCF_{fish} (L/kg, FW tissue)	—	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.30E+05
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	5.00E-04
Oral CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997b)	C-1-7	3.40E-01
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.80E-03
Inhalation URF (μg/m^3)$^{-1}$	U.S.EPA (1997b)	C-2-1	9.70E-05
Inhalation CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997c)	C-2-2	3.40E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-63

CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	278.34
T_m (K)	Montgomery and Welkom (1991)	--	238.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	5.55E-08 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.08E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.43E-06
D_a (cm²/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.38E-02
D_w (cm²/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	7.86E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.25E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.57E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.57E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.18E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.27E+01
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.11E+01

CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.989393
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.01E+03
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	6.43E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	7.24E-02
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	7.24E-02
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.16E+03
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.16E+03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.17E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.32E-03

CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
	Biotransfer Factors for Animals (Continued)		
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.60E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.17E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	1.04E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.58E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
	Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-01
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	3.50E-01
Inhalation URF (μg/m³)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYLPHTHALATE (117-84-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	390.56
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	248.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	5.90E-09 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.00E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.68E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.32E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.20E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.14E+09
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.03E+08
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.03E+06
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.78E+07
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.61E+07

TABLE A-3-64

CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYLPHTHALATE (117-84-0)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.55E+06
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.93E-01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.57E-04
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.57E-04
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.28E+08
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.28E+08

TABLE A-3-64

CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYLPHTHALATE (117-84-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.70E+01
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.37E+01
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	6.50E+01
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.70E+04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.24E+01
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.88E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997a)	C-1-8	2.00E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.00E-02
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	304.36
T_m (K)	Howard (1989-1993)	--	393.1
Vp (atm)	Vp value cited in Howard (1989-1993).	--	1.11E-07 at 25°C (solid)
S (mg/L)	S value cited in Howard (1989-1993).	--	6.88E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.89E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.71E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.24E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	6.46E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.33E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.33E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.96E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.31E+02

CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	--	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	ND
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999382
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	2.06E+02
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.55E+00
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.43E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.43E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.31E+03
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.31E+03

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.13E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.62E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.96E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.13E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.28E-04
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). The geometric mean value was obtained from various literature sources (see Appendix A3.4).	B-4-26	4.63E+02
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were obtained from U.S. EPA (1995b). OR Default BAF value recommended for use by U.S. EPA (1995b), when literature data were not available	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	9.00E-04
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.15E-03
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-66

CHEMICAL-SPECIFIC INPUTS FOR DIBENZ(A,H)ANTHRACENE (53-70-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	278.33
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	539.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.70E-14 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	6.70E-04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.12E-08
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.80E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	6.01E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.53E+06
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	--	1.79E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.79E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.34E+05
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	7.16E+04

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.69E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.010868
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.56E+04
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.43E-04
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.36E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.36E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.68E+07
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.68E+07

TABLE A-3-66

CHEMICAL-SPECIFIC INPUTS FOR DIBENZ(A,H)ANTHRACENE (53-70-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.80E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.86E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.07E-01
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.80E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (5.8/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	7.00E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.28E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	Calculated by multiplying the Oral CSF for Benzo(a)pyrene by the relative potency factor for Dibenz(a,h)anthracene of 1.0 (U.S.EPA 1993e).	C-1-7	7.30E+00
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	2.10E-03
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	7.30E+00

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	236.36
T_m (K)	Montgomery and Welkom (1991)	--	279.2
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	1.0E-03 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	1.20E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.97E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.79E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.79E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	2.19E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.47E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.47E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.10E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.79E+00

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999999
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.10E+01
$Br_{root\ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.22E+01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.72E+00
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.72E+00
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	8.81E-02
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	8.81E-02

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.74E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.50E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	6.65E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.74E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.34E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.54E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1996d)	C-1-8	5.70E-05
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-1-7	1.40E+00
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	2.00E-04
$Inhalation\ URF$ (μg/m^3)$^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	4.00E-04
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	U.S.EPA (1996d)	C-2-2	2.40E-03

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-68

CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	208.3
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	252.1
Vp (atm)	Vp value cited in Montgomery and Weldom (1991).	--	2.00E-02 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	3.44E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.21E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.96E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.05E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994g).	--	1.50E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	7.05E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.05E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.29E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.82E+00

CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.73E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.45E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.14E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.14E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	9.59E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	9.59E-03

CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.19E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.77E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.56E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.19E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.97E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980) (see Appendix A-3).	B-4-26	2.65E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	8.40E-02
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.00E-02
$Inhalation\ URF$ (μg/m^3)$^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	2.4E-05
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	8.4E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	147.01
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	256.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.79E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.25E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.11E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.11E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.93E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.79E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	3.79E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.79E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.84E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.52E+01

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay and others (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.11E+02
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.92E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.95E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.95E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.24E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.24E-01

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.21E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.00E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	8.48E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.21E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.53E-05
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.45E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	9.00E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997c)	C-2-3	2.00E-01
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	147.01
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	297.86
Vp (atm)	Vp value cited in Howard (1989-1993).	--	3.03E-03 at 25°C (solid)
S (mg/L)	S value cited in Howard (1989-1993).	--	6.88E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.11E+02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.14E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.85E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	3.39E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	8.03E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.03E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.02E+02

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.21E+02
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.28E+02
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.59E+00
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.53E-01
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.53E-01
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	8.02E-02

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} $\left(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	8.02E-02
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.69E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.52E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.03E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.69E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	6.72E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.84E+02
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	8.90E-02
Oral CSF (mg/kg/day)$^{-1}$	—	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	3.12E-01
Inhalation URF (µg/m³)$^{-1}$	—	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	—	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	147.01
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	326.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.39E-03 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.30E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.80E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.14E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.85E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	2.58E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	6.16E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.16E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.62E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.46E+01

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.05E+02
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.70E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.13E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.13E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	8.60E-02
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	8.60E-02

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.05E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.49E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.86E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.05E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.12E-05
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.31E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1996c)	C-1-8	2.30E-01
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	2.40E-02
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	8.00E-01
Inhalation URF (μg/m^3)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	6.90E-03
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	2.40E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-72

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DICHLOROBENZIDINE (91-94-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	253.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	405.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.89E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.52E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.08E-08
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.28E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.48E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.76E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	8.70E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.70E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.52E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.48E+01

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DICHLOROBENZIDINE (91-94-1)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.847495
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.38E+02
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.58E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.32E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.32E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.73E+04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.73E+04

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DICHLOROBENZIDINE (91-94-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.99E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	9.44E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.14E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.99E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	7.45E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.07E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	NA
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	4.50E-01
RfC (mg/m^3)	--	C-2-3	NA
Inhalation URF (μg/m^3)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	1.30E-04
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	4.50E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR DICHLORODIFLUOROMETHANE (75-71-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	120.92
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	115.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	6.40E+00 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	3.0E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.58E+00
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.77E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	9.00E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.44E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	6.85E+0
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.85E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.14E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.74E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.70E+01
$Br_{rootveg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.48E+01
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.19E+00
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.19E+00
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.33E-06
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.33E-06

CHEMICAL-SPECIFIC INPUTS FOR DICHLORODIFLUOROMETHANE (75-71-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.15E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.63E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	4.40E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.15E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	2.87E-06
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.58E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.00E-01
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997c)	C-2-3	2.00E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHANE (75-34-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	98.97
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	175.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	3.0E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	5.16E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.75E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.42E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.05E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	6.20E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	5.30E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.98E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.12E+00

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHANE (75-34-3)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.643
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \; DW \; plant}{\mu g/mL \; soil \; water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.19E+01
$Br_{rootveg}$ $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.24E+01
Br_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.56E+00
Br_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.56E+00
Bv_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	7.88E-04
Bv_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	7.88E-04

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.93E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.56E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.89E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.92E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	1.23E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.36E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	1.00E-01
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1995b)	C-1-7	9.1-E-02
RfC (mg/m³)	U.S. EPA (1997c)	C-2-3	5.00E-01
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	2.60E-05
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	9.1-E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-75

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (107-06-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	98.96
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	233.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.07E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	8.31E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.27E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.19E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.10E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.90E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.96E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.96E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.47E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	7.83E-01

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (107-06-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.41E+00
$Br_{rootveg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.81E+01
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.53E+00
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.53E+00
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.58E-03
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.58E-03

TABLE A-3-75

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (107-06-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.30E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.28E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	8.82E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.30E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.75E-07
BCF_{fish} (L//kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	7.61E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1996b)	C-1-8	2.90E-03
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	9.10E-02
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.00E-02
Inhalation URF (μg/m³)$^{-1}$	U.S. EPA (1997b)	C-2-1	2.60E-05
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-2-2	9.10E-02

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	96.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	150.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	7.88E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.0E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.55E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.53E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.09E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.32E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	6.50E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.50E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.88E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.60E+00

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.63E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.50E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.30E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.30E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.98E-04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.98E-04

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.05E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.32E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	4.01E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.05E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	2.62E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.41E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	9.00E-03
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	6.00E-01
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	3.20E-02
Inhalation URF (μg/m³)$^{-1}$	U.S. EPA (1997b)	C-2-1	5.00E-05
Inhalation CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997c)	C-2-2	1.80E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	--	96.94
T_m (K)	Howard (1989-1993)	--	192.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.30E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	4.94E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.51E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.36E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.13E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	9.60E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.98E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.98E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.73+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.99E+01

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.41E+01
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.38E+00
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.77E+00
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.77E+00
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.60E-03
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.60E-03

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.63E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.41E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.92E-06
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.63E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.90E-06
BCF_{fish} (unitless, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.89E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	3.50E-02
$Inhalation\ URF$ (μg/m³)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-78

CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	96.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	223.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	4.63E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	6.03E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.44E-03
D_a (cm²/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.16E-02
D_w (cm²/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	9.75E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	9.60E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	3.80E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.80E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.85E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.52E+00
ksg (year)[-1]	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	1.000000

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.41E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.71E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.77E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.77E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	9.70E-04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	9.70E-04
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.63E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.41E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.92E-06
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.63E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.90E-06

TABLE A-3-78

CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.89E+01
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—.	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.0E-02
Oral CSF (mg/kg/day)$^{-1}$	—	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E-02
Inhalation URF (μg/m^3)$^{-1}$	—	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	—	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-79

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	163.01
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	318.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	7.21E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	4.93E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.38E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.69E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.79E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	1.09E+03
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH $\quad$ K_{oc} 1 $\quad$ 159.0 2 $\quad$ 159.0 3 $\quad$ 159.0 4 $\quad$ 159.0 5 $\quad$ 158.8 6 $\quad$ 156.8 7 $\quad$ 139.6 8 $\quad$ 67.31 9 $\quad$ 12.75 10 $\quad$ 3.50 11 $\quad$ 2.51 12 $\quad$ 2.41 13 $\quad$ 2.40 14 $\quad$ 2.40
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.05E+01

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.58E+00
ksg (year)⁻¹	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999948
Biotransfer Factors for Plants			
RCF $\cdot \frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	5.68E+01
$Br_{root\ veg}$ $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.07E+01
Br_{ag} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.82E-01
Br_{forage} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.82E-01
Bv_{ag} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.01E+02
Bv_{forage} $\left(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.01E+02

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	8.62E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.73E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.30E-05
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	8.62E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.15E-05
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.19E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-03
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.1E-02
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-80

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROPROPANE (78-87-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	112.99
T_m (K)	Montgomery and Welkom (1991)	--	172.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	6.66E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.68E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.81E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.21E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.71E-06
K_{sw} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.78E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	4.70E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.53E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.88E+00
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.96E-01

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROPROPANE (78-87-5)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
	Biotransfer Factors for Plants		
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.89E+01
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3)	B-2-10	4.01E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.94E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.94E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.96E-03
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.96E-03

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.41E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.47E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	5.41E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.41E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	3.53E-06
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were obtained from U.S. EPA (1995b).	B-4-26	3.02E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1996c)	C-1-8	1.10E-03
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c))	C-1-7	6.80E-02
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	4.00E-03
Inhalation URF (μg/m^3)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	1.90E-05
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	6.80E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,3-DICHLOROPROPENE (542-75-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	110.98
T_m (K)	Montgomery and Welkom (1991)	--	189.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	4.11E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.55E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.94E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.26E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.00E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	5.60E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.70E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.03E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.08E+00
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.24E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	1.000000

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,3-DICHLOROPROPENE (542-75-6)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.15E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.25E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.78E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.78E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.38E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.38E-03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.45E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.41E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.70E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.45E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.11E-06

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,3-DICHLOROPROPENE (542-75-6)

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Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.25E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-04
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1995b)	C-1-7	1.8E-01
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	2.0E-02
Inhalation URF (μg/m^3)$^{-1}$	U.S. EPA (1997c)	C-2-1	3.70E-05
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	1.3E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	220.98
T_m (K)	--	--	NA
Vp (atm)	Vp value cited in Howard (1989-1993).	--	6.93E-05 at 25°C (liquid)
S (mg/L)	S value cited in Howard (1989-1993).	--	1.6E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.57E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.32E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.33E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	2.69E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.85E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.85E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.38E+00

CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	7.38E-01
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	1.49E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999991
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.24E+00
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.00E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.78
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.78
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.95-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.95-03

TABLE A-3-82

CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.14E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.76E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	8.18E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.14E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.33E-07
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	7.19E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-04
$Oral\ CSF$ $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	2.9E-01
RfC (mg/m³)	U.S. EPA (1997b)	C-2-3	5.00E-04
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	8.3E-05
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	2.9E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	380.93
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	449.1
Vp (atm)	Vp value cited in U.S. EPA (1992a)	--	1.72E-12 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1992a)	--	1.87E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.51E-09
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.36E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	4.29E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	1.86E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.55E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.55E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.91E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.02E+03

CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	2.34E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.082830
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.66E+03
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.04E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.49E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.49E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for above ground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.50E+06
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for abovegound produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.50E+06

CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.48E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.67E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	5.65E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.48E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.68E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.86E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	5.00E-05
Oral CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997b)	C-1-7	1.60E+01
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.80E-04
Inhalation URF (μg/m^3)$^{-1}$	U.S.EPA (1997b)	C-2-1	4.60E-03
Inhalation CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997c)	C-2-2	1.6-E+01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-84

CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	222.24
T_m (K)	Montgomery and Welkom (1991)	--	232.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.17E-06 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	8.80E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.48E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.56E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.35E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.73E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	8.20E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.15E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.28E+00
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.52E+00

CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999726
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.12E+02
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	7.46E+02
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.06E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.06E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.42E+03
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.42E+03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.17E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.87E-04

TABLE A-3-84

CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	8.31E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.17E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	5.42E-04
BCF_{fish} (L/kg FW tissue)	—	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	2.45E+03
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	8.00E-01
Oral CSF (mg/kg/day)$^{-1}$	—	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	2.80E+00
Inhalation URF (μg/m³)$^{-1}$	—	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	—	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	194.19
T_m (K)	Montgomery and Welkom (1991)	--	273.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.17E-06 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	4.19E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.01E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.96E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.13E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	4.30E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.66E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.66E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.00E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.06E+01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999726
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.05E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.95E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.40E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.40E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.05E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.05E+01

CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.42E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.08E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.31E-06
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.42E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	8.53E-07
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.03E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	1.00E+01
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	NA
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.50E+01
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	NA
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	NA

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Moses (1978)	--	122.17
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	300.1
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	2.18E-07 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1992a).	--	6.25E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.27E-09
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.84E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.69E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	2.29E+02
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH K_{oc} 1 126.0 2 126.0 3 126.0 4 126.0 5 126.0 6 125.99 7 125.9 8 125.02 9 116.87 10 71.06 11 15.77 12 3.43 13 2.05 14 1.91
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.26E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.44E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.04E+00
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.997404
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.16E+01
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.71E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.68E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-8	1.68E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.27E+03

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.27E+03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.82E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.75E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	6.96E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.82E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.54E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.66E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

(Page 4 of 4)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.00E-02
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-87

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DIMETHYOXYBENZIDINE (119-90-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	244.28
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	410.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	3.30E-10 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	2.40E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.36E-10
D_a (cm²/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.38E-02
D_w (cm²/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	5.60E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	6.46E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.65E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.65E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.74E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.46E+00

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DIMETHYOXYBENZIDINE (119-90-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.876710
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.21E+01
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.30E+01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.48E+00
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.48E+00
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.41E+04
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.41E+04

TABLE A-3-87

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DIMETHYOXYBENZIDINE (119-90-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.13E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.62E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.96E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.13E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.28E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.40E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-1-7	1.40E-02
RfC (mg/m³)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m³)$^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	4.0E-03
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	1.40E-02

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-88

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	168.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	363
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f).	--	4.0E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f).	--	5.4E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.25E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.18E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	9.15E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994f).	--	3.10E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.06E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.06E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.55E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.25E-01

TABLE A-3-88

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999661
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \; DW \; plant}{\mu g/mL \; soil \; water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.58E+00
$Br_{rootveg}$ $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.64E+01
Br_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.32E+00
Br_{forage} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.32E+00
Bv_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, C. Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.74E+01
Bv_{forage} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.74E+01

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.46E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.79E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	9.43E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.46E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	6.15E-07
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	7.40E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-04
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.50E-04
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

(Page 1 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	184.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	385.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.52E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	5.8E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.82E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.06E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.30E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH K_{oc} 1 0.80 2 0.79 3 0.72 4 0.38 5 0.08 6 0.02 7 0.01 8 0.01 9 0.01 10 0.01 11 0.01 12 0.01 13 0.01 14 0.01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.0E-04 (at pH 7.0)

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

(Page 2 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	7.5E-04 (at pH 7.0)
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	4.0E-04 (at pH 7.0)
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.62E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999461
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.74E+00
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 in Appendix A-3).	B-2-10	9.74E+04
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.13E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.13E+00

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.80E+02
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vight (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.80E+02
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.62E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.29E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.00E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.62E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	6.54E-07
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	8.40E+00
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA

TABLE A-3-89

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

(Page 4 of 4)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-03
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E-03
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-90

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROTOLUENE (121-14-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Howard (1989-1993)	--	182.14
T_m (K)	Howard (1989-1993)	--	344
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.29E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.85E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.46E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.09E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	7.86E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	9.90E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.10E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.10E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.83E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.04E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999088
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.43E+01
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.80E+01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.72E+00
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.72E+00
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.10E+01
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.10E+01

TABLE A-3-90

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROTOLUENE (121-14-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.86E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.49E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.01E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.86E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.96E-06
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	5.92E+00
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless, FW tissue)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1995d)	C-1-8	2.0E-03
$Oral\ CSF$ (mg/kg/day)$^{-1}$	The $Oral\ CSF$ value represents a 2,4/2,6-Dinitrotoluene mixture (U.S. EPA 1997b).	C-1-7	6.8E-01
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E-03
$Inhalation\ URF$ (μg/m^3)$^{-1}$	—	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	6.8E-01

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Howard (1989-1993)	--	182.15
T_m (K)	Howard (1989-1993)	--	339
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	7.47E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.05E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.30E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.11E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	7.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	7.70E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.19E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.19E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.14E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.68E+00

TABLE A-3-91

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999686
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.29E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.08E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.15E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.15E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.41E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.41E+01

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.12E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.93E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.34E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.12E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.53E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	5.92E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-03
$Oral\ CSF$ (mg/kg/day)$^{-1}$	The $Oral\ CSF$ value represents a 2,4/2,6-Dinitrotoluene mixture (U.S. EPA 1997b).	C-1-7	6.8E-01
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.5E-03
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-2-2	6.8E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DIOXANE (123-91-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	88.10
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	284.9
Vp (atm)	Vp value cited in U.S. EPA (1995b)	--	5.00E-02 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b)	--	9.00E+05
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.89E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.20E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.05E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	--	5.40E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	8.76E-01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.76E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.57E-02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.50E-02

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.45E+00
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	7.37E+02
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.53E+01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.53E+01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.93E-03
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.93E-03

TABLE A-3-92

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DIOXANE (123-91-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.29E-09
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.36E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.64E-08
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.29E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.07E-08
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.69E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	1.1E-02
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	3.1E-06
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIPHENYLHYDRAZINE (122-66-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	184.24
T_m (K)	Montgomery and Welkom (1991)	--	401.1
Vp (atm)	Vp value cited in U.S. EPA (1995b)	--	4.74E-08 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b)	--	6.80E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.28E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.95E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.24E-06
K_{ow} (unitless)	Montgomery and Welkom (1991)	--	8.71E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.78E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.78E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.09E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.11E+01

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIPHENYLHYDRAZINE (122-66-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.998800
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.90E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.76E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	7.74E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	7.74E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.89E+02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.89E+02

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.92E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.19E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.65E-05
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.92E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.73E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.01E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	8.0E-01
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	U.S. EPA (1997b)	C-2-1	2.2E-04
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	8.0E-01

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-94

CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	274.38
T_m (K)	T_m value cited in U.S. EPA (1995b).	--	248
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	3.7E-07 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	1.6E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.12E-06
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.50E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	5.21E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	9.55E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.80E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.80E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction oF 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.35E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	7.20E+01

CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.20E+01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.998394
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.76E+02
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.55E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.94E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.94E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.35E+02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.35E+02

TABLE A-3-94

CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.59E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.40E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.90E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.59E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.89E-04
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.23E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	4.00E-05
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.40E-04
Inhalation URF ($\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-95

CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	406.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	343.1
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	1.72E-11 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1992a).	--	2.31E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.04E-08
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.59E-03
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.02E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.04E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.04E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.53E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.16E+01
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.78E+01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	0.074720

CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\cdot\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}\cdot$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.17E+02
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.75E+00
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.77E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.77E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	9.36E+03
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	9.36E+03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.40E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.59E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	9.18E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.40E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.99E-05

CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.60E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	6.00E-03
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.10E-02
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	380.93
T_m (K)	U.S.EPA (1992a)	--	473.1
Vp (atm)	Vp value cited in U.S. EPA (1992a)	--	7.68E-10 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1992a)	--	2.46E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.19E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.07E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	5.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	7.79E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.08E+08
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.08E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.11E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.32E+02

CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+04
Fv (unitless)	--	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.563463
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent	B-2-10	1.36E+03
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.26E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.76E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.76E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	7.62E+03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	7.62E+03

CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.19E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.96E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.37E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.19E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.55E-03
BCF_{fish} (L/kg, FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	BAFs were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. BCFs were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). FCMs were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	8.55E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	3.00E-04
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.10E-03
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (106-89-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	92.53
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	247.5
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	2.20E-02 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	6.60E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.08E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.13E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.10E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.78E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.22E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.22E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.66E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.88E-02

CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (106-89-8)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.67E+00
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.00E+02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.77E+01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.77E+01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.35E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.35E-03

CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (106-89-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.41E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.47E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	5.41E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.41E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.53E-08
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	9.13E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1995b)	C-1-8	2.00E-03
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	9.90E-03
RfC (mg/m³)	U.S. EPA (1997b)	C-2-3	1.00E-03
Inhalation URF (μg/m³)$^{-1}$	U.S. EPA (1997b)	C-2-1	1.20E-06
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	4.20E-03

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-98

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	MW value cited in U.S. EPA (1995b)	--	114.14
T_m (K)	--	--	NA
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	2.30E-02 at 25°C
S (mg/L)	S value cited in U.S. EPA (1995b).	--	1.90E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.38E-04
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.07E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	9.35E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	3.89E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.46E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.46E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.85E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	9.80E-01

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value cited in NC DEHNR (1997).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.02E+01
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.14E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.67E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.67E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.00E-02
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.00E-02

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.09E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	9.77E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.18E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.09E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	7.71E-07
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	9.51E+00
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	9.00E-02
Oral CSF (mg/kg/day)$^{-1}$	—	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	3.20E-01
Inhalation URF (μg/m³)$^{-1}$	—	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	—	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	124.15
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	373.0
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	3.50E-04 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	4.90E+05
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.87E-08
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.63E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	8.84E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.12E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.55E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.55E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.16E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.19E-02

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.88E+01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.56E+00
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	4.24E+02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.63E+01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.63E+01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	7.11E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	$Bv_{leafyveg}$ value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	7.11E-01

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	8.90E-09
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2..81E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	3.41E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	8.90E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	2.22E-08
BCF_{fish} (L/kg, FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.42E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1995b)	C-1-7	2.93E+02
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	8.4E+01
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	2.93E+02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-100

CHEMICAL-SPECIFIC INPUTS FOR ETHYLBENZENE (100-41-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.16
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.26E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.73E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.73E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.65E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.49E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.33E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.04E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.04E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.53E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.16E+00

CHEMICAL-SPECIFIC INPUTS FOR ETHYLBENZENE (100-41-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	2.53E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.52E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.20E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.07E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.07E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.53E-02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.53E-02

TABLE A-3-100

CHEMICAL-SPECIFIC INPUTS FOR ETHYLBENZENE (100-41-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.05E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.33E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.03E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.05E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.63E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.39E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-01
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	1.00E+00
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE DIBROMIDE (106-93-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	187.88
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	282.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	1.00E-02 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	4.20E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.47E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.17E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.19E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	5.62E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.28E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.28E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.46E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.31E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.15E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.50E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.77E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.77E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	9.13E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	9.13E-03

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE DIBROMIDE (106-93-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.47E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.41E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.71E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.47E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.12E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.26E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1996c)	C-1-8	5.70E-05
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	8.50E+01
RfC (mg/m^3)	U.S. EPA (1995b)	C-2-3	2.00E-04
Inhalation URF (μg/m^3)$^{-1}$	U.S. EPA (1997b)	C-2-1	2.20E-04
Inhalation CSF (mg/kg/day)$^{-1}$	Calculated from Inhalation URF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-2	7.70E-01

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-102

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE OXIDE (75-21-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	44.05
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	162.1
Vp (atm)	Verschueren (1983)	--	1.44E+00 at 25°C (liquid)
S (mg/L)	S value cited in NC DEHNR (1996).	--	3.80E+05
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.67E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.71E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.44E-05
K_{sw} (unitless)	Howard (1989-1993)	--	5.01E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	8.26E-01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.26E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.19E-02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.30E-02
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.13E+01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
F_v (unitless)	F_v value was calculated by using the equation cited in Junge (1977). Recommended value of F_v was calculated by using the V_p value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.44E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	7.80E+02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.77E+01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.77E+01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.60E-04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.60E-04
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.98E-09
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.26E-08

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE OXIDE (75-21-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.52E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.98E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	9.94E-09
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.48E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-1-7	1.02E+00
RfC (mg/m³)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997c)	C-2-1	1.0E-04
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-2-2	3.5E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-103

CHEMICAL-SPECIFIC INPUTS FOR BIS(2-ETHYLHEXYL)PHTHALATE (117-81-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	390.54
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	218.1
Vp (atm)	Vp value cited in Montgomery and Welkom (1991).	--	1.12E-11 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1992a).	--	3.96E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.10E-08
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.32E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.22E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.60E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.11E+09
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.11E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.33E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.44E+03

CHEMICAL-SPECIFIC INPUTS FOR BIS(2-ETHYLHEXYL)PHTHALATE (117-81-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.10E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.37E+03
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.13E+00
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.80E-02
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.80E-02
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.77E+06
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.77E+06

CHEMICAL-SPECIFIC INPUTS FOR BIS(2-ETHYLHEXYL)PHTHALATE (117-81-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.27E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.03E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.88E-03
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.27E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.18E-03
BCF_{fish} (L/kg, FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.60E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S.EPA (1997b)	C-1-7	1.40E-02
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.00E-02
$Inhalation\ URF$ (μg/m^3)$^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	4.00E-06
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	1.4E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	202.26
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	383.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.07E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.32E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.33E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.75E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.18E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	1.21E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	4.91E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.91E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.68E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.96E+03

CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	5.75E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.992042
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.92E+03
$Br_{root\ veg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.90E+00
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.46E-02
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.46E-02
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.56E+03
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.56E+03

CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.65E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.05E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.69E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.65E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.41E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	BAFs were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. BCFs were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). FCMs were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.57E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	4.0E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.4E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	166.22
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	389.1
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	1.08E-09 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1992a).	--	1.90E+00
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.41E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.63E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	7.88E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	--	1.47E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	7.71E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.71E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction oF 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.78E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.08E+02

TABLE A-3-105

CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.22E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.934896
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.83E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.96E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.51E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.51E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.63E+04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.63E+04

CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.17E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.70E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.48E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.17E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.92E-04
BCF_{fish} (L/kg FW tissue)	---	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.20E+03
$BSAF_{fish}$ (unitless)	---	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	4.00E-02
Oral CSF (mg/kg/day)$^{-1}$	---	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.40E-01
Inhalation URF (μg/m^3)$^{-1}$	---	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	---	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-106

CHEMICAL-SPECIFIC INPUTS FOR FORMALDEHYDE (50-00-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	30.03
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	365.1
Vp (atm)	Vp value cited in U.S. EPA (1994c)	--	5.10E+00 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b)	--	5.50E+05
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.78E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.00E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	1.74E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	--	2.20E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.62E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.62E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.96E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.05E-01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.73E+00
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.57E+02
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.46E+01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for above ground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.46E+01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.65E-04
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.65E-04

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.75E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.53E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	6.69E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.75E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.36E-08
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	1.07E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-01
Oral CSF $(mg/kg/day)^{-1}$	Calculated from Inhalation URF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-1-7	4.50E-02
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.00E-01
Inhalation URF $(\mu g/m^3)^{-1}$	U.S.EPA (1997b)	C-2-1	1.30E-05
Inhalation CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997c)	C-2-2	4.50E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1995b)	--	46.03
T_m (K)	U.S. EPA (1995b)	--	282.0
Vp (atm)	Vp value cited in U.S. EPA (1995b)	--	5.40E-02 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b)	--	1.00E+06
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.49E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.22E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.71E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	--	2.90E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.39E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.39E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.04E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.16E-01

CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	6.40E+00
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.19E+02
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	7.92E+01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	7.92E+01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.02E-03
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.02E-03

CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.30E-09
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.28E-09
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	8.82E-09
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.30E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.75E-09
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.30E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	2.00E+00
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.00E+00
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-108

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)DIOXIN (35822-46-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	425.31
T_m (K)	U.S. EPA (1994a)	--	537.1
Vp (atm)	U.S. EPA (1994a)	--	4.22E-14 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	2.40E-06
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.50E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.11E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.89E-06
K_{ow} (unitless)	U.S. EPA (1992d)	--	1.58E+08
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.77E+07
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.77E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.33E+06
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.91E+06

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)DIOXIN (35822-46-9)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.09E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.016157
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.79E+05
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.90E-01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	7.05E-04
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	7.05E-04
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	3.50E+05
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	3.50E+05

TABLE A-3-108

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)DIOXIN (35822-46-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.4E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-03
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	2.55E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	8.58E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	5.00E-03
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.01
Health Benchmarks			
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-8	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)FURAN (67562-39-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	409.31
T_m (K)	U.S. EPA (1994a)	--	509.1
Vp (atm)	U.S. EPA (1994a)	--	1.75E-13 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	1.35E-06
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.30E-05
D_a (cm²/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.55E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.99E-06
K_{ow} (unitless)	U.S. EPA (1992d)	--	8.32E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.13E+07
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.13E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.85E+06
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.05E+06

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)FURAN (67562-39-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.034709
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.91E+05
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.68E-01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.02E-03
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.02E-03
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.40E+05
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.40E+05

TABLE A-3-109

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)FURAN (67562-39-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-03
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	2.09E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	7.04E-03
BCF_{fish} (L/kg FW tissue)	---	B-4-26	NA
BAF_{fish} (L/kg FW)	---	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	5.00E-03
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.01
Health Benchmarks			
Oral CSF (mg/kg/day)$^{-1}$	---	C-1-8	ND
Inhalation CSF (mg/kg/day)$^{-1}$	---	C-1-7	ND
RfD (mg/kg/day)	---	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	---	C-2-1	ND
RfC (mg/m^3)	---	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-110

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,7,8,9-HEPTACHLORODIBENZO(P)FURAN (55673-89-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	409.31
T_m (K)	U.S. EPA (1994a)	--	494.1
Vp (atm)	U.S. EPA (1994a)	--	1.41E-13 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	1.40E-06
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.30E-05
D_a (cm²/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.55E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.99E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	--	8.32E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.13E+07
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.13E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.85E+06
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.05E+06

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,7,8,9-HEPTACHLORODIBENZO(P)FURAN (55673-89-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.020142
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.91E+05
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.68E-01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.02E-03
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.02E-03
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.40E+05
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.40E+05

**CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,7,8,9-HEPTACHLORODIBENZO(P)FURAN (55673-89-7)**

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	3.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	1.63E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	1.97E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	2.42E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	1.06E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	5.00E-03
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.01
Health Benchmarks			
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-8	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	373.35
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	368.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	4.29E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.73E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.87E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.12E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.69E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.04E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	9.53E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.53E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.15E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.81E+02

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999718
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	–	1.70E+03
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.78E+01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.89E-02
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.89E-02
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.09E+03
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.09E+03

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	8.22E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.60E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	3.15E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	8.22E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	2.05E-03
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	5.52E+03
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	4.50E+00
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.80E-03
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997b)	C-2-1	1.30E-03
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-2-2	4.50E+00

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-112

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	389.32
T_m (K)	Montgomery and Welkom (1991)	--	430.1
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	7.51E-12 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1992a) .	--	2.68E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.09E-08
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.32E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	4.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.62E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	7.18E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.18E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.38E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.87E+02

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	4.58E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.203415
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.06E+03
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.48E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.96E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.96E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.86E+05
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.86E+05

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.47E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.41E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.71E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.47E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.12E-03
BCF_{fish} (L/kg FW tissue)	—	B-4-26	NA
BAF_{fish} (L/kg FW)	BAFs were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. BCFs were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). FCMs were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.88E+03
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	1.30E-05
Oral CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997b)	C-1-7	9.1E+00
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	4.6E-05
Inhalation URF (μg/m^3)$^{-1}$	U.S.EPA (1997b)	C-2-1	2.6E-03
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	9.1E+00

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,7,8-HEXACHLORODIBENZO(P)DIOXIN (39227-28-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	390.87
T_m (K)	U.S. EPA (1994a)	--	546.1
Vp (atm)	U.S. EPA (1994a)	--	1.33E-13 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	4.40E-06
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.20E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.15E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.12E-06
K_{ow} (unitless)	U.S. EPA (1992d)	--	6.17E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.80E+07
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.80E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.85E+06
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.52E+06

TABLE A-3-113

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,7,8-HEXACHLORODIBENZO(P)DIOXIN (39227-28-6)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.09E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.059645
Biotransfer Factors for Plants			
RCF $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}\right)$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.31E+05
$Br_{rootveg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	6.09E-01
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.22E-03
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.22E-03
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.50E+05
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.50E+05

**CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,7,8-HEXACHLORODIBENZO(P)DIOXIN (39227-28-6)**

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	6.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	3.26E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.94E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	4.53E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	4.03E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.10
Health Benchmarks			
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-8	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-114

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,6,7,8-HEXACHLORODIBENZO(P)DIOXIN (57653-85-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	390.87
T_m (K)	U.S. EPA (1994a)	--	558.1
Vp (atm)	U.S. EPA (1994a)	--	4.74E-14 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	4.40E-06
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.20E-05
D_a (cm²/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDD.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.15E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.12E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	--	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.10E+07
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,6,7,8-HEXACHLORODIBENZO(P)DIOXIN (57653-85-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.39E+05
ksg (year)⁻¹	ksg value assumed to be the same as the ksg value calculated for 1,2,3,4,7,8-HexaCDD. ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.09E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.028857
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	8.10E-01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.50E-03
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.50E-03
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.50E+05
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.50E+05

TABLE A-3-114

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,6,7,8-HEXACHLORODIBENZO(P)DIOXIN (57653-85-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	5.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	2.71E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.29E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	3.70E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	2.57E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.10
Health Benchmarks			
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-8	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8,9-HEXACHLORODIBENZO(P)DIOXIN (19408-74-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	390.87
T_m (K)	U.S. EPA (1994a)	--	516.1
Vp (atm)	U.S. EPA (1994a)	--	6.45E-14 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	4.40E-06
H (atm·m^3/mol)	U.S.EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.20E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.15E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.12E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1994a).	--	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.10E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.39E+05

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8,9-HEXACHLORODIBENZO(P)DIOXIN (19408-74-3)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was assumed to be the same as the ksg value for 1,2,3,4,7,8-HexaCDD. ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.09E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.015299
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	8.10E-01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.50E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.50E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.50E+05
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.50E+05

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8,9-HEXACHLORODIBENZO(P)DIOXIN (19408-74-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	5.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	2.71E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.29E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	2.33E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	1.39E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.10
Health Benchmarks			
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-8	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-116

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,7,8-HEXACHLORODIBENZO(P)FURAN (70648-26-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	374.87
T_m (K)	U.S. EPA (1994a)	--	498.6
Vp (atm)	U.S. EPA (1994a)	--	3.16E-13 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	8.25E-06
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.40E-05
D_a (cm²/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.62E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.23E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d)	--	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.10E+07
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,7,8-HEXACHLORODIBENZO(P)FURAN (70648-26-9)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.39E+05
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.048600
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	8.10E-01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.50E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.50E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.50E+05
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.50E+05

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,7,8-HEXACHLORODIBENZO(P)FURAN (70648-26-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	7.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	3.80E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	4.60E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	4.51E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	3.48E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.10
Health Benchmarks			
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-117

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,6,7,8-HEXACHLORODIBENZO(P)FURAN (57117-44-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	374.87
T_m (K)	U.S. EPA (1994a)	--	505.1
Vp (atm)	U.S. EPA (1994a)	--	2.89E-13 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	1.77E-05
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.10E-06
D_a (cm²/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.62E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.23E-06
K_{ow} (unitless)	Homologue groupaverage value obtained from U.S. EPA (1992d)	--	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.10E+07
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.39E+05

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,6,7,8-HEXACHLORODIBENZO(P)FURAN (57117-44-9)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.051501
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	8.10E-01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.50E-03
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.50E-03
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.50E+05
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.50E+05

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,6,7,8-HEXACHLORODIBENZO(P)FURAN (57117-44-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	6.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	3.26E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.94E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	4.53E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	3.56E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.10
Health Benchmarks			
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-8	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-118

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8,9-HEXACHLORODIBENZO(P)FURAN (72918-21-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	374.87
T_m (K)	U.S. EPA (1994a)	--	519.1
Vp (atm)	U.S. EPA (1994a)	--	2.37E-13 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	1.30E-05
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.00E-05
D_a (cm²/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.62E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.23E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	--	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.10E+07
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05

**CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8,9-HEXACHLORODIBENZO(P)FURAN (72918-21-9)**

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.39E+05
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.057593
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	8.10E-01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.50E-03
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.50E-03
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.50E+05

TABLE A-3-118

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8,9-HEXACHLORODIBENZO(P)FURAN (72918-21-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotranfer Factors for Plants (Continued)			
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.50E+05
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	6.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	3.26E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.94E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	ND
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.10
Health Benchmarks			
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-8	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

TABLE A-3-119

CHEMICAL-SPECIFIC INPUTS FOR
2,3,4,6,7,8-HEXACHLORODIBENZO(P)FURAN (60851-34-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	374.87
T_m (K)	U.S. EPA (1994a)	--	512.1
Vp (atm)	U.S. EPA (1994a)	--	2.63E-13 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	1.30E-05
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.00E-05
D_a (cm²/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.62E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.23E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	--	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.10E+07
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.22E+05

CHEMICAL-SPECIFIC INPUTS FOR
2,3,4,6,7,8-HEXACHLORODIBENZO(P)FURAN (60851-34-5)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.39E+05
ksg (year)⁻¹	Ksg value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.054727
Biotransfer Factors for Plants			
RCF ($\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$)	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.88E+04
$Br_{rootveg}$ ($\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil}$)	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	8.10E-01
Br_{ag} ($\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil}$)	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.50E-03
Br_{forage} ($\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil}$)	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.50E-03
Bv_{ag} ($\frac{\mu g/g \ DW \ plant}{\mu g/g \ air}$)	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.50E+05
Bv_{forage} ($\frac{\mu g/g \ DW \ plant}{\mu g/g \ air}$)	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.50E+05

TABLE A-3-119

CHEMICAL-SPECIFIC INPUTS FOR
2,3,4,6,7,8-HEXACHLORODIBENZO(P)FURAN (60851-34-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	5.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	2.71E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	3.29E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	2.11E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	1.74E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	4.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.10
Health Benchmarks			
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-8	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-120

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE (PERCHLOROBUTADIENE) (87-68-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	260.76
T_m (K)	Montgomery and Welkom (1991)	--	252.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.33E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.54E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.39E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.73E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.33E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.38E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	6.94E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.94E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.20E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.77E+02

**CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE
(PERCHLOROBUTADIENE) (87-68-3)**

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999997
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.03E+03
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.48E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	7.14E-02
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	7.14E-02
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.55E-01
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.55E-01

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE (PERCHLOROBUTADIENE) (87-68-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.28E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.35E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.64E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.27E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.07E-03
BCF_{fish} (L/kg FW tissue)	—	B-4-26	NA
BAF_{fish} (L/kg FW)	BAFs were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. BCFs were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). FCMs were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.69E+03
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1995b)	C-1-8	2.00E-04
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	7.80E-02
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	7.00E-04
Inhalation URF (μg/m³)$^{-1}$	U.S. EPA (1997b)	C-2-1	2.20E-05
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	7.80E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-121

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	284.8
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	504.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	1.62E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	8.62E-03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.35E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.41E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	B-4-20	7.84E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.18E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	8.00E+04
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.00E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.00E+03
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.20E+03

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Cemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.21E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999663
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.02E+03
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.02E+00
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.56E-02
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.56E-02
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	7.57E+01
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	7.57E+01

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.53E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.993E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	9.68E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.53E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	6.31E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—see Appendix A-3.	B-4-27	5.52E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	8.0E-04
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	1.6E+00
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.8E-03
$Inhalation\ URF$ (μg/m^3)$^{-1}$	U.S. EPA (1997b)	C-2-1	4.6E-04
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	1.6E+00

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-122

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	272.77
T_m (K)	Montgomery and Welkom (1991)	--	264.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	9.63E-05 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.53E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.72E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.61E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.21E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	8.07E_04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.51E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.51E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.13E+2
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.80E+02

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999994
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.40E+03
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.47E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.65E-02
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.65E-02
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.47E-01
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.47E-01

TABLE A-3-122

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.41E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.03E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	2.45E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.41E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	1.60E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	5.25E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	7.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997c)	C-2-3	7.00E-05
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, Heckelman (1989)	--	236.74
T_m (K)	Montgomery and Welkom (1991)	--	459.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	6.21E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	4.08E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.60E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.77E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.88E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	9.66E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.82E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.82E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.36E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	7.27E+01

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.78E+02
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	1.53E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{leafveg}$ value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.93E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.93E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	$Bv_{leafveg}$ value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990; 1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-9	2.72E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1990; 1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-9	2.72E-01

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.67E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.43E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	2.94E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.67E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	1.92E-04
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	6.29E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.00E-03
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	1.40E-02
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.50E-03
$Inhalation\ URF$ (μg/m^3)$^{-1}$	U.S. EPA (1997b)	C-2-1	4.00E-06
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	1.40E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith and Heckleman (1989)	--	406.92
T_m (K)	Budavari, O'Neil, Smith and Heckleman (1989)	--	437.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	3.60E-15 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	3.0E-03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.88E-10
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.46E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.01E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	3.47E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.08E+06
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.08E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.08E+04
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.31E+04

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.71E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000143
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.49E+05
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	1.38E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.70E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.70E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.23E+10
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.23E+10

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.75E-01
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.71E-01
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	1.05E+00
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.75E+02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-14	6.88E-01
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.66E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.00E-04
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.10E-03
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR HYDROGEN CHLORIDE (7647-01-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	36.47
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	158.9
Vp (atm)	U.S. EPA (1994b)	--	4.6E+01 (liquid)
S (mg/L)	--	--	ND
H (atm·m³/mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.73E-01
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	2.00E-05
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	--	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	ND
Kd_{sw} (L/Kg)	--	B-4-16; B-4-18; B-4-24	ND
Kd_{bs} (mL/g)	--	B-4-16; B-4-25	ND
ksg (year)⁻¹	--	B-1-2; B-2-2; B-3-2; B-4-2	ND
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000

CHEMICAL-SPECIFIC INPUTS FOR HYDROGEN CHLORIDE (7647-01-0)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ WW\ plant}{\mu g/mL\ soil\ water}$	--	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	--	B-2-10	ND
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	--	B-2-9	ND
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	--	B-3-9	ND
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	--	B-2-8	NA
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	--	B-3-8	NA
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	--	B-3-11	ND
Ba_{beef} (day/kg FW)	--	B-3-10	ND
Ba_{pork} (day/kg FW)	--	B-3-12	ND
BCF_{egg} (day/kg FW)	--	B-3-13	ND
BCF_{chick} (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW)	--	B-4-26	ND
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

CHEMICAL-SPECIFIC INPUTS FOR HYDROGEN CHLORIDE (7647-01-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			
RfD (mg/kg/day)	Calculated from *RfC* using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-1-8	5.7E-03
Oral CSF (mg/kg/day)⁻¹	--	C-1-7	ND
RfC (mg/m³)	U.S. EPA (1997b)	C-2-3	2.0E-02
Inhalation URF (μg/m³)⁻¹	--	C-2-1	ND
Inhalation CSF (mg/kg/day)⁻¹	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-126

CHEMICAL-SPECIFIC INPUTS FOR INDENO(1,2,3-CD)PYRENE (193-39-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	276.34
T_m (K)	Montgomery and Welkom (1991)	--	435
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	1.88E-13 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.07E-02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.86E-09
D_a (cm²/s)	D_a value was obtained from WATER8 model database U.S. EPA (1995d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.90E-02
D_w (cm²/s)	D_w value was obtained from WATER8 model database U.S. EPA (1995d)	B-4-20	5.66E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	8.22E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.11E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.11E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.08E+05
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.64E+05

CHEMICAL-SPECIFIC INPUTS FOR INDENO(1,2,3-CD)PYRENE (193-39-5)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.47E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.007092
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.91E+04
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.19E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.90E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.90E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.67E+08
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.67E+08

TABLE A-3-126

CHEMICAL-SPECIFIC INPUTS FOR INDENO(1,2,3-CD)PYRENE (193-39-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.53E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.07E-01
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.50E-01
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.53E+01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.63E-01
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.31E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	Calculated by multiplying the *Oral CSF* for Benzo(a)pyrene by the relative potency factor for Indeno(1,2,3-cd)pyrene of 0.1 (U.S.EPA 1993e).	C-1-7	7.3E-01
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	Calculated from *Oral CSF* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	2.1E-04
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	C-2-2	7.3E-01

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-127

CHEMICAL-SPECIFIC INPUTS FOR ISOPHORONE (78-59-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	138.21
T_m (K)	Montgomery and Welkom (1991)	--	265.1
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	7.08E-07 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.20E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.15E-09
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.22E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.50E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.00E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.99E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.99E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.25E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.20E+00

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Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.10E+01
$Br_{rootveg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.68E+01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.04E+00
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.04E+00
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.42E+02
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.42E+02

CHEMICAL-SPECIFIC INPUTS FOR ISOPHORONE (78-59-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.97E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.26E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.52E-06
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.97E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	9.92E-07
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow}, obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.15E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.00E-01
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S.EPA (1997b)	C-1-7	9.50E-04
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.00E-01
$Inhalation\ URF$ (μg/m^3)$^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	2.70E-07
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	9.50E-04

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-128

CHEMICAL-SPECIFIC INPUTS FOR LEAD (7439-92-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	207.2
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	600.5
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.43E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	6.28E-06
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from Baes, Sharp, Sjoreen, and Shor (1984), which states that several factors, such as experimental methods and soil type, could influence partitioning or Kd_s values. Baes, Sharp, Sjoreen, and Shor (1984) compares values between various literature sources and provide this value, which is based on its best judgment.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.00E+02
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	9.00E+02
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	9.00E+02
ksg (year)⁻¹	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties (Continued)		
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000
	Biotransfer Factors for Plants		
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	--	B-2-10	ND
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{root\ veg}$.	B-2-10	9.00E-03
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	1.36E-02
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Bv values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{forage}.	B-3-8	4.50E-02
Br_{grain} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{grain} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{grain}.	B-3-8	9.00E-03
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

CHEMICAL-SPECIFIC INPUTS FOR LEAD (7439-92-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	2.5E-04
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	3.0E-04
Ba_{pork} (day/kg FW)	NC DEHNR (1997)	B-3-12	3.6E-04
Ba_{egg} (L/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	--	B-4-26	ND
BAF_{fish} (day/kg FW)	Because lead is hydrophobic, BAF was used. BAF_{fish} value was obtained from NC DEHNR (1997).	B-4-27	8.0
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR MALATHIONE (121-75-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	330.36
T_m (K)	Montgomery and Welkom (1991)	--	276
Vp (atm)	Vp value cited in Howard (1989-1993).	--	1.04E-08 at 25°C (liquid)
S (mg/L)	S value cited in Howard (1989-1993).	--	1.43E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.40E-08
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.47E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.29E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	2.29E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.81E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.81E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.36E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.92E+00

CHEMICAL-SPECIFIC INPUTS FOR MALATHIONE (121-75-5)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.945884
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.16E+01
$Br_{root \ veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.20E+01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.68E+00
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.68E+00
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	7.58E+02
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	7.58E+02

CHEMICAL-SPECIFIC INPUTS FOR MALATHIONE (121-75-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.82E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.75E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	6.96E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.82E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.54E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.66E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E-02
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-130

CHEMICAL-SPECIFIC INPUTS FOR MERCURIC CHLORIDE (7487-94-7)

(Page 1 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	271.52
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	550.1
Vp (atm)	U.S. EPA (1996a)	--	1.20E-04
S (mg/L)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	6.90E+04
H (atm·m³/mol)	U.S. EPA (1997g)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.1E-10
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1997g).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.53E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	5.25E-06
K_{ow} (unitless)	U.S. EPA (1996a)	--	6.10E-01
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	U.S. EPA (1997g)	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.80E+04
Kd_{sw} (L/Kg)	U.S. EPA (1997g)	B-4-16; B-4-18; B-4-24	1.00E+05
Kd_{bs} (mL/g)	U.S. EPA (1997g)	B-4-16; B-4-25	5.00E+04
ksg (year)$^{-1}$	U.S. EPA (1996a)	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Estimated based on discussions concerning divalent mercury provided in U.S. EPA (1996a).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.850000

CHEMICAL-SPECIFIC INPUTS FOR MERCURIC CHLORIDE (7487-94-7)

(Page 2 of 4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\left(\dfrac{\mu g/g \ WW \ plant}{\mu g/mL \ soil \ water}\right)$	---	B-2-10	ND
$Br_{rootveg}$ $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil}\right)$	U.S. EPA (1997g)	B-2-10	3.60E-02
Br_{ag} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil}\right)$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	1.45E-02
Br_{forage} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil}\right)$	U.S. EPA (1997g)	B-3-9	0.0
Bv_{ag} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air}\right)$	U.S. EPA (1997g)	B-2-8	1.8E+03
Bv_{forage} $\left(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air}\right)$	U.S. EPA (1997g)	B-3-8	1.8E+03

CHEMICAL-SPECIFIC INPUTS FOR MERCURIC CHLORIDE (7487-94-7)

(Page 3 of 4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Default Ba_{milk} (dry weight value) obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 87% moisture content in milk. U.S. EPA U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated Ba_{milk} (wet weight) value was multiplied by 0.87.	B-3-11	2.26E-03
Ba_{beef} (day/kg FW)	Default Ba_{beef} (dry weight value) obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 70% moisture content in beef. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated Ba_{beef} (wet weight) value was multiplied by 0.87.	B-3-10	5.22E-03
Ba_{pork} (day/kg FW)	Default Ba_{pork} (dry weight value) of 0.00013 day/kg DW btained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 70 % moisture content in pork. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated Ba_{pork} (wet weight) value was multiplied by 0.87.	B-3-12	3.39E-05
Ba_{egg} (day/kg FW)	Default Ba_{egg} (dry weight value) of 0.11 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 75 % moisture content in eggs. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated Ba_{egg} (wet weight) value was multiplied by 0.87.	B-3-13	2.39E-02
$Ba_{chicken}$ (day/kg FW)	Default $Ba_{chicken}$ (dry weight value) of 0.11 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 75 % moisture content in chicken. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{chicken}$ (wet weight) value was multiplied by 0.87.	B-3-14	2.39E-02
BCF_{fish} (L/kg FW)	—	B-4-26	NA
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	3.0E-04
$Oral\ CSF$ (mg/kg/day)$^{-1}$	—	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.1E-03

CHEMICAL-SPECIFIC INPUTS FOR MERCURIC CHLORIDE (7487-94-7)

(Page 4 of 4)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks (Continued)			
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR MERCURY (7439-97-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	200.59
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	234.23
Vp (atm)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	2.63E-06 at 25°C
S (mg/L)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	5.62E-02
H (atm·m³/mol)	U.S. EPA (1997g)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.1E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate D_a values. A density value of 13.546 g/cc for mercury was used.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.09E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate D_w values. A density value of 13.546 g/cc for mercury was used.	B-4-20	3.01E-05
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	U.S.EPA (1997g)	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.00E+03
Kd_{sw} (L/Kg)	U.S.EPA (1997g)	B-4-16; B-4-18; B-4-24	1.00E+03
Kd_{bs} (mL/g)	U.S.EPA (1997g)	B-4-16; B-4-25	3.00E+03
ksg (yr)$^{-1}$	U.S. EPA (1996a)	B-1-2; B-2-2; B-3-2; B-4-2	0.0

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999774
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	--	B-2-10	ND
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Elemental mercury does not deposit onto soils. Therefore, it is assumed that there is no plant uptake through the soil.	B-2-10	NA
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	NA
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Elemental mercury is assumed not to deposit onto soils. Therefore, it is assumed that there is no transfer of mercury to the aboveground plant parts through root uptake.	B-3-8	NA
Br_{grain} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Elemental mercury is assumed not to deposit onto soils. Therefore, it is assumed that there is no transfer of mercury to the aboveground plant parts through root uptake.	B-3-8	NA
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Elemental mercury exists in very low concentrations in the vapor phase. Therefore, Bv_{ag} value for elemental mercury is not modeled for the indirect exposure pathways. Elemental mercury is modeled for the inhalation pathway only. No literature data is available to calculate a Bv_{ag} value for elemental mercury.	B-2-8	ND
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Elemental mercury exists in very low concentrations in the vapor phase. Therefore, Bv_{forage} value for elemental mercury is not modeled for the indirect exposure pathways. Elemental mercury is modeled for the inhalation pathway only. No literature data is available to calculate a Bv_{forage} value for elemental mercury.	B-3-8	ND

CHEMICAL-SPECIFIC INPUTS FOR MERCURY (7439-97-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Elemental mercury does not deposit onto soils nor gets transferred to the aboveground plant parts. Therefore, there is no transfer of elemetal mercury into the animal tissue.	B-3-11	NA
Ba_{beef} (day/kg FW)	Elemental mercury does not deposit onto soils nor gets transferred to the aboveground plant parts. Therefore, there is no transfer of elemetal mercury into the animal tissue.	B-3-10	NA
Ba_{pork} (day/kg FW)	Elemental mercury does not deposit onto soils nor gets transferred to the aboveground plant parts. Therefore, there is no transfer of elemetal mercury into the animal tissue.	B-3-12	NA
Ba_{egg} (day/kg FW)	Elemental mercury does not deposit onto soils nor gets transferred to the aboveground plant parts. Therefore, there is no transfer of elemetal mercury into the animal tissue.	B-3-13	NA
$Ba_{chicken}$ (day/kg FW)	Elemental mercury does not deposit onto soils nor gets transferred to the aboveground plant parts. Therefore, there is no transfer of elemetal mercury into the animal tissue.	B-3-14	NA
BCF_{fish} (L/g FW tissue)	—	B-4-26	NA
BAF_{fish} (L/kg FW)	Elemental mercury does not deposit onto soils and surface water. Therefore, there is no transfer of elemetal mercury into the fish tissue.	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	Calculated from RfC using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-1-8	8.60E-05
$Oral\ CSF$ (mg/kg/day)$^{-1}$	—	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	3.0E-04
$Inhalation\ URF$ (μg/m^3)$^{-1}$	—	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	—	C-2-2	ND

Note:

NA = Not available
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	67.09
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	237.3
Vp (atm)	Vp value cited in U.S. EPA (1995b)	--	8.90E-02 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b)	--	2.50E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.39E-04
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.15E-01
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.33E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	3.47E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.74E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.74E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.80E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.49E-01

CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be zero due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\cdot \dfrac{\mu g/g \; DW \; plant}{\mu g/mL \; soil \; water} \cdot$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.91E+00
$Br_{rootveg}$ $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.85E+02
Br_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.89E+01
Br_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.89E+01
Bv_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	8.81E-04
Bv_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	8.81E-04

CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.76E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.72E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.06E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.76E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	6.88E-08
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.52E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997c)	C-2-3	7.0E-04
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-133

CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	32.04
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	175.3
Vp (atm)	Vp value cited in Montgomery and Welkom (1991)	--	1.30E-01 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b)	--	2.90E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.44E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.58E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.64E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	1.95E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.96E-01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.96E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.97E-02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.58E-02
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that	B-1-1; B-2-1; B-2-7; B-2-8;	1.000000

CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

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Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.37E+00
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.61E+03
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	9.96E+01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	9.96E+01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.82E-05
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.82E-05
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.30E-09
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.30E-09
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	5.21E-09
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.55E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.39E-09

CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.70E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-01
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.8E+00
$Inhalation\ URF$ ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-134

CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	345.65
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	351.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.62E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	8.84E-02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.33E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.30E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.59E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	3.36E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	8.00E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.00E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.00E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.20E+03

TABLE A-3-134

CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	6.93E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.901041
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \; DW \; plant}{\mu g/mL \; soil \; water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-10	7.16E+02
$Br_{rootveg}$ $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	8.95E-01
Br_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	9.38E-02
Br_{forage} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	9.38E-02
Bv_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.83E+02
Bv_{forage} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.83E+02

CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.67E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.43E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	1.02E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.67E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	6.66E-04
BCF_{fish} (L/kg, FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.16E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.00E-03
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.80E-02
Inhalation URF (μg/m³)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-135

CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	--	74.08
T_m (K)	Montgomery and Welkom (1991)	--	175.1
Vp (atm)	Vp value cited in Howard (1989-1993).	--	2.84E-01 at 25°C (liquid)
S (mg/L)	S value cited in Howard (1989-1993).	--	2.44E+05
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.64E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.23E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.10E-05
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	2.90E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.25E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.25E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.44E-01

CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.30E-01
ksg (year)$^{-1}$	Ksg value assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.84E+00
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.10E+02
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.09E+01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.09E+01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.01E-03
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.01E-03

CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.30E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.28E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	8.82E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.30E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	5.75E-08
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.32E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	1.00E+00
Oral CSF (mg/kg/day)$^{-1}$		C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.50E+01
Inhalation URF (μg/m^3)$^{-1}$		C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$		C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR METHYL BROMIDE (74-83-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith and Heckelman (1989)	--	94.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	179.44
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.16E+00 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.45E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.41E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.28E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.21E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.30E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	9.00E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.00E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.75E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.60E-01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.98E+00
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	8.87E+01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.79E+00
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.79E+00
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.07E-05
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.07E-05

CHEMICAL-SPECIFIC INPUTS FOR METHYL BROMIDE (74-83-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.03E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.27E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	3.95E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.03E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	2.58E-07
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.14E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.40E-03
$Oral\ CSF$ $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	5.00E-03
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR METHYL CHLORIDE (74-87-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	50.49
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	176.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	5.68E+00 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	6.34E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.52E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.13E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.39E-05
K_{sw} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	8.00E+00
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	6.00E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.00E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.50E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.40E-01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boehling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.46E+00
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	1.24E+02
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.16E+01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.16E+01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.13E-05
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.13E-05

TABLE A-3-137

CHEMICAL-SPECIFIC INPUTS FOR METHYL CHLORIDE (74-87-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.36E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.01E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	2.43E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.35E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	1.59E-07
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.86E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	Calculated from RfC using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-1-8	8.60E-02
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1995c)	C-1-7	1.30E-02
RfC (mg/m³)	U.S.EPA (1997d)	C-2-3	3.00E-01
Inhalation URF (μg/m³)$^{-1}$	U.S. EPA (1995b)	C-2-1	1.80E-06
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1995b)	C-2-2	6.30E-03

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	72.10
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	187.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	1.20E-01 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	2.40E+05
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.61E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.35E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.03E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.91E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.34E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.34E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.76E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	9.36E-02

CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.69E+00
$Br_{rootveg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.86E+02
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.67E+01
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.67E+01
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.08E-03
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.08E-03

TABLE A-3-138

CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.51E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.79E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	5.79E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.51E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	3.78E-08
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	9.61E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	6.00E-01
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	1.00E+00
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-139

CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	100.16
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	188.4
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	2.50E-02 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	2.00E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.25E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.59E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.36E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.55E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.20E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.00E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.80E-01

CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.22E+00
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	6.85E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	7.95E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	7.95E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	8.26E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	8.26E-03

CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.23E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.89E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.71E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.23E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.07E-07
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—see Appendix A-3.	B-4-26	4.73E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	8.0E-02
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997a)	C-1-7	8.0E-01
RfC (mg/m^3)	U.S. EPA (1995b)	C-2-3	8.0E-02
Inhalation URF (μg/m^3)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	2.3E-01
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	8.0E-01

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1997g)	--	216.0
T_m (°K)	--	--	ND
Vp (atm)	--	--	ND
S (mg/L)	--	--	ND
H (atm·m^3/mol)	U.S. EPA (1997g)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.7E-07
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1997g).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.28E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	6.11E-06
K_{ow} (unitless)	--	--	ND
K_{oc} (mL/g)	--	--	ND
Kd_s (mL/g)	U.S. EPA (1997g)	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.00E+03
Kd_{sw} (L/Kg)	U.S. EPA (1997g)	B-4-16; B-4-18; B-4-24	1.00E+05
Kd_{bs} (mL/g)	U.S. EPA (1997g)	B-4-16; B-4-25	3.00E+03
ksg (year)$^{-1}$	U.S. EPA (1996a)	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Based on discussions provided in U.S. EPA (1996a), methyl mercury does not exist in the air/vapor phase.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	--	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	U.S. EPA (1997g)	B-2-10	9.9E-02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	2.94E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	U.S. EPA (1997g)	B-3-9	0.0
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Methyl mercury is assumed not to exist in the air phase. Therefore, there is no biotransfer of methyl mercury from air into plants.	B-2-8	NA
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Methyl mercury is assumed not to exist in the air phase. Therefore, there is no biotransfer of methyl mercury from air into plants.	B-3-8	NA
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Default Ba_{milk} (dry weight value) of 0.02 day/kg DW for mercury obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 87% moisture content in milk. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated Ba_{milk} (wet weight) value was multiplied by 0.13.	B-3-11	3.38E-04
Ba_{beef} (day/kg FW)	Default Ba_{beef} (dry weight value) of 0.02 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 70% moisture content in beef. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated Ba_{beef} (wet weight) value was multiplied by 0.13.	B-3-10	7.80E-04

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
Ba_{pork} (day/kg FW)	Default Ba_{pork} (dry weight value) of 0.00013 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 70 % moisture content in pork. U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated Ba_{pork} (wet weight) value was multiplied by 0.13.	B-3-12	5.07E-06
Ba_{egg} (day/kg FW)	Default Ba_{egg} (dry weight value) of 0.11 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 75 % moisture content in eggs.U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated Ba_{egg} (wet weight) value was multiplied by 0.13.	B-3-13	3.58E-03
$Ba_{chicken}$ (day/kg FW)	Default $Ba_{chicken}$ (dry weight value) of 0.11 day/kg DW obtained from U.S. EPA (1997g) was converted to a wet weight basis assuming a 75 % moisture content in chicken.U.S. EPA (1997g) does not differentiate between different forms of mercury. Mercury is assumed to be in the form of 87% divalent mercury and 13% methyl mercury in herbivore animals. Therefore, the calculated $Ba_{chicken}$ (wet weight) value was multiplied by 0.13.	B-3-14	3.58E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	Default value cited in U.S. EPA (1997g) for a Trophic Level 4 fish.	B-4-27	6.80E+06
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-04
$Oral\ CSF$ $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.5E-04
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-141

CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	263.23
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	310.1
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	1.30E-08 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1992a).	--	5.00E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.84E-08
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.87E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.43E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	--	7.20E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.40E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.80E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	9.59E+00

CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.966349
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.31E+01
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.80E+01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.64E-01
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.64E-01
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	9.02E+02
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	9.02E+02

CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.72E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.81E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.19E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.72E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.43E-05
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	8.74E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.54E-04
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	8.8E-04
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	173.86
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	220.4
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	2.20E+00 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	1.45E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.64E-02
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.10E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	7.06E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	4.17E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.60E-01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.60E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.95E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.04E+00

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.04E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	4.01E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.48E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.48E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.13E-04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.13E-04

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.31E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.05E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	1.27E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.31E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	8.27E-07
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.00E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	1.0E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.5E-02
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-143

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	84.94
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	4.87E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.74E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.38E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.69E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.25E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.80E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.00E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.00E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.50E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.00E-01

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.46E+00
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	8.46E+01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	7.29E+00
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	7.29E+00
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.11E-04
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.11E-04

TABLE A-3-143

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.43E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.52E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	5.47E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.43E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	3.57E-07
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.30E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	6.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	7.5E-03
RfC (mg/m³)	U.S. EPA (1997c)	C-2-3	3.0E+00
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997b)	C-2-1	4.7E-07
Inhalation CSF $(mg/kg/day)^{-1}$	Calculated from the Inhalatioin URF using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-2	1.6E-03

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-144

CHEMICAL-SPECIFIC INPUTS FOR NAPHTHALENE (91-20-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	128.16
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	353.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.17E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.11E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.82E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.26E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	B-4-20	8.92E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.36E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.19E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.19E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.93E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.76E+01
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	5.27E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999999
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.81E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	8.23E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.35E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.35E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.52E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.52E-01

CHEMICAL-SPECIFIC INPUTS FOR NAPHTHALENE (91-20-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.87E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.92E-05
Biotransfer Factors for Animals (Continued)			
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.16E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.87E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.67E-05
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.15E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1995b)	C-1-8	4.0E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.40E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-145

CHEMICAL-SPECIFIC INPUTS FOR NICKEL (7440-02-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	58.69
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	1,828
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.26E-01
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.46E-05
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
ksg (year)⁻¹	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

CHEMICAL-SPECIFIC INPUTS FOR NICKEL (7440-02-0)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
F_V (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	--	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	8.00E-03
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value for fruits was calculated by multiplying the uptake slope factor with a conversion factor of 2 x10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1993e) for garden fruits. Br_{ag} value for vegetables was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2 x10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1993e). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	9.31E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-8	3.20E-02
Br_{grain} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{grain} value was calculated by multiplying the uptake slope factors with a conversion factor of 2 x 10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals.	B-3-8	6.00E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

TABLE A-3-145

CHEMICAL-SPECIFIC INPUTS FOR NICKEL (7440-02-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	1.0E-03
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	6.0E-03
Ba_{pork} (day/kg FW)	--	B-3-12	ND
Ba_{egg} (day/kg FW)	--	B-3-13	NA
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	NA
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-3-26	3.07E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, FW tissue)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-02
$Oral\ CSF$ $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.02E-02
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROANILINE (88-74-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	342.1
Vp (atm)	Vp value cited in Montgomery and Welcom (1991).	--	1.07E-05 at 25°C (solid)
S (mg/L)	S value cited in Montgomery and Welcom (1991).	--	1.26E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.17E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.29E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.81E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	7.08E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.93E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.93E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.95E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.57E+01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999980
Biotransfer Factors for Plants			
RCF $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}\right)$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.25E+01
$Br_{root\ veg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.18E+00
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.30E+00
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.30E+00
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.47E+00
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.47E+00

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROANILINE (88-74-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.62E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.78E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.15E-06
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.62E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.40E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.50E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	6.00E-05
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	NA
RfC (mg/m^3)	U.S. EPA (1997c)	C-2-3	2.00E-04
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	NA
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	NA

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	387.1
Vp (atm)	--	--	1.07E-05 at 25°C (solid)
S (mg/L)	S value cited in Montgomery and Welcom (1991)	--	8.90E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.65E-06
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.11E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	8.23E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	2.34E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.66E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.66E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.24E+01

CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.62E+00
ksg (year)⁻¹	Ksg value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999993
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	8.94E+00
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.40E+00
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.26E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.26E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	9.71E-01

CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	9.71E-01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.86E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.88E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.12E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.86E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.64E-07
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—see Appendix A-3.	B-4-26	5.92E+00
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	3.00E-03
Oral CSF (mg/kg/day)$^{-1}$	—	C-1-7	NA
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.05E-02
Inhalation URF (µg/m³)$^{-1}$	—	C-2-1	NA
Inhalation CSF (mg/kg/day)$^{-1}$	—	C-2-2	NA

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	419.10
Vp (atm)	--	--	ND
S (mg/L)	S value cited in Montgomery and Welcom (1991)	--	1.07E-05
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.65E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.31E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.75E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	2.46E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.72E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.72E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.29E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.89E+00

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999944
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g \; DW \; plant}{\mu g/mL \; soil \; water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	9.04E+00
$Br_{root \; veg}$ $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{root \; veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.25E+00
Br_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.08E+00
Br_{forage} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.08E+00
Bv_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.02E+00
Bv_{forage} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.02E+00

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.95E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.18E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.48E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.95E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.88E-07
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.00E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	3.00E-03
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	NA
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.05E-02
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	NA
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	NA

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-149

CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	123.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	279.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	3.21E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.92E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.06E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.43E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	9.43E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	6.80E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.19E+02
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.19E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.93E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.76E+004

CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.28E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the liquid-phase Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999998
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.23E+01
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.03E+01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.38E+00
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.38E+00
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.43E-01
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.43E-01

CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.40E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.71E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.07E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.40E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.35E-06
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)—See Appendix A-3.	B-4-26	5.92E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	2.0E-03
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-150

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	139.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	317.1
Vp (atm)	Vp value cited in Howard (1989-1993).	--	2.63E-04 at 25°C (solid)
S (mg/L)	S value cited in Howard (1989-1993).	--	2.50E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.46E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.44E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.19E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	6.17E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.53E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.53E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.65E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.41E+01

TABLE A-3-150

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999999
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.19E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.36E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.57E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.57E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.08E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.08E-01

A-3-520

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.90E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.55E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.88E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.90E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.22E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.35E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-151

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	139.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	386.1
Vp (atm)	Vp value cited in Howard (1989-1993).	--	1.32E-06 at 25°C (solid)
S (mg/L)	S value cited in Howard (1989-1993).	--	2.50E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.32E-09
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.30E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.61E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	8.13E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.37E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.37E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.28E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.75E+01

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	2.09E+02
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999939
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.32E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.01E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.05E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.05E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	8.26E+02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	8.26E+02

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.46E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.04E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.47E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.46E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.61E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.67E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	6.20E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	NA
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.17E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	NA
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	NA

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-152

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	MW value cited in U.S. EPA (1995b)	--	158.20
T_m (K)	--	--	NA
Vp (atm)	Vp value cited in U.S. EPA (1995b)	--	3.80E-04 at 25°C
S (mg/L)	S value cited in U.S. EPA (1995b)	--	1.10E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.47E-05
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.50E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	7.52E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	2.57E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.07E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10;B-3-3; B-3-4; B-3-5; B-3-6;B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.07E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.05E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.29E+00

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.44E+00
Fv (unitless)	Fv value cited in NC DEHNR (1997).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.30E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.14E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.57E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.57E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.77E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.77E-01

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.04E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.46E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.82E-06
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.04E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.10E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.00E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	5.4E+00
RfC (mg/m^3)	--	C-2-3	ND
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	U.S. EPA (1997b)	C-2-1	1.6E-03
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-2-2	5.4E+00

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-153

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	198.23
T_m (K)	Montgomery and Welkom (1991)	--	339.6
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	1.74E-07 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1992a).	--	3.50E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.84E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.12E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.35E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.06E+03
K_{oc} (mL/g)	Estimated value was obtained from U.S. EPA (1994c).	--	3.27E+02, for pH range of 4.9 to 8.0
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.27E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.45E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.31E+01

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.44E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.998671
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	5.61E+01
$Br_{root \ veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.71E+01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.89E-01
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.89E-01
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	9.51E+01
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	9.51E+01

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	8.45E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.67E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.24E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	8.45E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.11E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.18E+02
BAF_{fish} (L/kg, FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	—	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997b)	C-1-7	4.9E-03
RfC (mg/m³)	—	C-2-3	ND
Inhalation URF (μg/m³)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	1.4E-06
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	4.9E-03

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-154

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	130.19
T_m (K)	--	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1992a).	--	6.09E-06 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1992a).	--	1.46E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.43E-08
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.67E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.75E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	--	2.40E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.70E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.28E+00

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.80E-01
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999902
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.99E+00
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.29E+01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.17E+00
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.17E+00
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.04E+01

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.04E+01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.91E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.03E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.30E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.91E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.76E-07
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.59E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)		C-1-8	ND
$Oral \ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	7.0E+00
RfC (mg/m^3)		C-2-3	ND
$Inhalation \ URF$ ($\mu g/m^3$)$^{-1}$	U.S. EPA (1997b)	C-2-1	2.0E-03
$Inhalation \ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-2-2	7.0E+00

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-155

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	460.76
T_m (K)	U.S. EPA (1994a)	--	598.1
Vp (atm)	U.S. EPA (1994a)	--	8.61E-11 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	4.00E-07
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.00E-09
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.06E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.69E-07
K_{ow} (unitless)	U.S. EPA (1994a)	--	3.89E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.40E+07
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.40E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.80E+06
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	9.60E+05

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CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.09E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.992606
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.62E+05
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	6.77E-01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.59E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.59E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	8.60E+06
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	8.60E+06
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-03

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-03
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	9.90E-03
$Ba_{chicken}$ (unitless, FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	1.10E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	1.00E-04
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.001
Health Benchmarks			
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-8	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-156

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	444.76
T_m (K)	U.S. EPA (1994a)	--	531.1
Vp (atm)	U.S. EPA (1994a)	--	4.93E-15 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	1.20E-06
H (atm·m³/mol)	U.S.EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.90E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.48E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.78E-06
K_{ow} (unitless)	U.S. EPA (1994a)	--	6.03E+08
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.72E+08
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.72E+06
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.79E+07
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.49E+07

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.10E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.001671
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g \; DW \; plant}{\mu g/mL \; soil \; water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.34E+06
$Br_{rootveg}$ $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.60E-01
Br_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.26E-04
Br_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.26E-04
Bv_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.30E+06
Bv_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.30E+06

TABLE A-3-156

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-03
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	7.92E-03
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (see Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	4.40E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	1.00E-04
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.001
Health Benchmarks			
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-157

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	356.42
T_m (K)	U.S. EPA (1994a)	--	513.1
Vp (atm)	U.S. EPA (1994a)	--	1.25E-12 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	1.20E-04
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.60E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.21E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.38E-06
K_{ow} (unitless)	U.S. EPA (1992d)	--	4.37E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.69E+06
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.69E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.02E+05
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.08E+05

**CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)**

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.219208
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.01E+04
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.12E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.62E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.62E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.20E+05
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.20E+05

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	4.71E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	5.50E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.50
Health Benchmarks			
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-8	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-158

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	340.42
T_m (K)	U.S. EPA (1994a)	--	498.1
Vp (atm)	U.S. EPA (1994a)	--	3.58E-12 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	2.40E-04
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.20E-06
D_a (cm²/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.70E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.51E-06
K_{ow} (unitless)	U.S. EPA (1992d)	--	6.17E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.80E+06
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.80E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.85E+05

**CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)**

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.52E+05
ksg (year)$^{-1}$	ksg value assumed to be the same as the ksg value calculated for 2,3,4,7,8-PentaCDF. ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.364027
Biotransfer Factors for Plants			
RCF $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}\right)$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.93E+04
$Br_{rootveg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.03E+00
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.61E-03
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.61E-03
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.60E+04
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.60E+04

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	2.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	1.09E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	1.31E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	ND
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.05
Health Benchmarks			
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-159

CHEMICAL-SPECIFIC INPUTS FOR
2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	340.42
T_m (K)	U.S. EPA (1994a)	--	469.1
Vp (atm)	U.S. EPA (1994a)	--	4.33E-12 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	2.36E-04
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.20E-06
D_a (cm²/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.70E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.51E-06
K_{ow} (unitless)	U.S. EPA (1992d)	--	8.32E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.13E+06
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.13E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.85E+05
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.05E+05

CHEMICAL-SPECIFIC INPUTS FOR
2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.263427
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.95E+04
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	9.65E-01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.87E-03
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.87E-03
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.60E+04
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.60E+04

TABLE A-3-159

CHEMICAL-SPECIFIC INPUTS FOR
2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	9.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	4.89E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	5.91E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	5.61E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	7.32E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.50
Health Benchmarks			
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
**Chemical/Physical Properties**			
MW (g/mole)	Montgomery and Welkom (1991)	--	250.34
T_m (K)	Montgomery and Welkom (1991)	--	358.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f)	--	3.10E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f)	--	3.20E-02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.43E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.86E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.34E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	1.22E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	3.21E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.21E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.41E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.29E+03

TABLE A-3-160

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.33E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999951
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.93E+03
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.99E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.44E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.44E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.04E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.04E-01

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.72E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.07E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.72E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.72E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.43E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.61E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	8.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	2.8E-03
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	295.36
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	417.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f). U.S. EPA (1994c) cites value from Howard (1989-1993)	--	3.1E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f); U.S. EPA (1994c) cites value from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	--	3.20E-02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt, (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.86E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.87E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	5.0E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994f).	--	4.37E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.89E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.89E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.42E+02
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.36E+02

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.62E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999987
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.75E+02
$Br_{root\,veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root\,veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.49E+01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.06E-02
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.06E-02
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.71E-01
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.71E-01

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.47E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.10E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.33E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.47E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	8.66E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.65E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	3.03E-03
$Oral\ CSF$ $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-1-7	2.6E-01
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.1E-02
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	7.4E-05
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	2.6E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

(Page 1 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	266.35
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	463
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	7.11E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.34E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.41E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.56E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	8.01E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.20E+05
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH K_{oc} 1 19,949 2 19,918 3 19,604 4 16,942 5 7,333 6 1,417 7 504.9 8 408.7 9 399.1 10 398.1 11 398.0 12 398.0 13 398.0 14 398.0
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	pH K_{oc} 1 199.5 2 199.2 3 196.0 4 169.4 5 73.33 6 14.17 7 5.05 8 4.09 9 3.99 10 3.98 11 3.98 12 3.98 13 3.98 14 3.98

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

(Page 2 of 4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	<table><tr><td>pH</td><td>K_{oc}</td></tr><tr><td>1</td><td>1,496</td></tr><tr><td>2</td><td>1,494</td></tr><tr><td>3</td><td>1,470</td></tr><tr><td>4</td><td>1,271</td></tr><tr><td>5</td><td>550.0</td></tr><tr><td>6</td><td>106.2</td></tr><tr><td>7</td><td>37.87</td></tr><tr><td>8</td><td>30.66</td></tr><tr><td>9</td><td>29.93</td></tr><tr><td>10</td><td>29.86</td></tr><tr><td>11</td><td>29.85</td></tr><tr><td>12</td><td>29.85</td></tr><tr><td>13</td><td>29.85</td></tr><tr><td>14</td><td>29.85</td></tr></table>
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	<table><tr><td>pH</td><td>K_{oc}</td></tr><tr><td>1</td><td>798.0</td></tr><tr><td>2</td><td>796.7</td></tr><tr><td>3</td><td>784.1</td></tr><tr><td>4</td><td>677.7</td></tr><tr><td>5</td><td>293.3</td></tr><tr><td>6</td><td>56.67</td></tr><tr><td>7</td><td>20.20</td></tr><tr><td>8</td><td>16.35</td></tr><tr><td>9</td><td>15.96</td></tr><tr><td>10</td><td>15.92</td></tr><tr><td>11</td><td>15.92</td></tr><tr><td>12</td><td>15.92</td></tr><tr><td>13</td><td>15.92</td></tr><tr><td>14</td><td>15.92</td></tr></table>
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.42E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999980
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.90E+03
$Br_{root\ veg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.77E+02
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.48E-02

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

(Page 3 of 4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Br_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.48E-02
Bv_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature(T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.02E+03
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.02E+03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.55E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.02E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.66E-03
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.55E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.39E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.97E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

(Page 4 of 4)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	3.0E-02
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	1.2E-01
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E-01
Inhalation URF (μg/m^3)$^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	3.4E-05
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on the Oral CSF assuming route-to-route extrapolation	C-2-2	1.2E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-163

CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	178.22
T_m (K)	Montgomery and Welkom (1991)	--	371.1
Vp (atm)	Geometric mean value calculated from values cited in Montgomery and Welkom (1991).	--	1.35E-03 at 25°C (solid)
S (mg/L)	S value cited in Lucius et al. (1992).	--	1.28E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.88E-01
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.33E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.47E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	3.55E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.01E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.01E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.76E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.01E+03
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.26E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7;	1.000000

CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	7.47E+02
$Br_{rootveg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.49E+00
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	9.08E-02
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	9.08E-02
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.08E-02
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.08E-02

CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.82E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.92E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.08E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.82E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	7.04E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	Default BAF value recommended for use by U.S. EPA (1995b), when literature data were not available.	B-4-27	3.30E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	NA
RfC (mg/m^3)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	NA
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	NA

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	94.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	314.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	5.74E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	9.08E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.95E-07
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.27E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.03E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	3.00E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH K_{oc} 1 22.0 2 22.0 3 22.0 4 22.0 5 22.0 6 22.0 7 22.0 8 21.8 9 20.0 10 11.2 11 2.27 12 0.51 13 0.32 14 0.30
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.65E+00

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.79E-01
ksg (year)⁻¹	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.53E+01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999999
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.50E+00
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-9; B-2-10; B-3-9	4.32E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.42E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-10	5.42E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-9	3.52E+00
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-9	3.52E+00

TABLE A-3-164

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.38E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.54E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	9.12E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.38E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.95E-07
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	7.81E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	6.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	2.1E+00
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	260.4
T_m (K)	--	--	ND
Vp (atm)	Vp value cited in Montgomery and Welkom (1991).	--	1.70E-06 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	3.80E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.16E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.05E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.88E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	6.46E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.33E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.33E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.96E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.31E+01

CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be zero due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999650
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.06E+02
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.55E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.43E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.43E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.48E+01
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.48E+01

CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.13E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.62E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.96E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.13E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.28E-04
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.63E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997c)	C-1-8	2.0E-04
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E-04
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-166

CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	148.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	403.9
Vp (atm)	Howard (1989-1993)	--	2.63E-07 at 25°C (solid)
S (mg/L)	Howard (1989-1993)	--	6.20E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.28E-09
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.04E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.97E-06
K_{sw} (unitless)	NC DEHNR (1997)	--	2.5E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.80E-01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.80E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.60E-02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.92E-02

CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.35E+04
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999797
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.39E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.33E+03
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.63E+01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.63E+01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.03E+00
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.03E+00

CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.99E-09
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.28E-09
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.60E-09
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.99E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.96E-09
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.05E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	2.0E+00
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997c)	C-2-3	1.2E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	256.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	428.1
Vp (atm)	Vp value cited in U.S. EPA (1995b)	--	5.30E-07 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b)	--	1.50E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.05E-06
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.71E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	5.45E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	3.24E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	7.74E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.74E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.81E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.10E+01

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999942
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.23E+02
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.59E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.62E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.62E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.38E+01
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.38E+01

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.57E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.13E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	9.84E-05
Ba_{egg} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.57E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	6.42E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.74E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	7.5E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.6E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-168

CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	202.24
T_m (K)	Montgomery and Welkom (1991)	--	429.1
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	7.36E-12 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1992a).	--	1.30E-01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.14E-08
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.72E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.14E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.00E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	6.80E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.80E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.10E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.72E+03

CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992)	B-1-2; B-2-2; B-3-2; B-4-2	1.33E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.196376
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.66E+03
$Br_{root\,veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\,veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.44E+00
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.98E-02
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.98E-02
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.04E+06
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.04E+06

CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.98E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.52E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.06E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.98E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.99E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	BAFs were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. BCFs were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). FCMs were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.19E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	3.0E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.1E-01
Inhalation URF (μg/m³)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	79.10
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	231.5
Vp (atm)	Vp value cited in U.S. EPA (1995b)	--	2.60E-02 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b)	--	3.00E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.86E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.10E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.08E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	4.68E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.72E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.72E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.54E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.89E-01

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}\right)$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.07E+00
$Br_{rootveg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.50E+02
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.59E+01
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.59E+01
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.22E-05
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.22E-05

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.72E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.18E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.42E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.72E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	9.28E-08
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.90E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-03
$Oral\ CSF$ $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	3.50E-03
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	321.57
T_m (K)	Montgomery and Welkom (1991)	--	314.1
Vp (atm)	--	--	ND
S (mg/L)	--	--	ND
H (atm·m³/mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.05E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.69E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	1.17E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.28E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.28E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.56E+02

CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.10E+03
ksg (year)⁻¹	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then ocnverted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.87E+03
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.46E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.55E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.55E-02
$Bv_{leafy\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$		B-2-8	ND
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$		B-3-8	ND

CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.33E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.95E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.57E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.33E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.33E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	BAFs were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. BCFs were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). FCMs were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.53E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	5.0E-02
Oral CSF (mg/kg/day)$^{-1}$		C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.8E-01
Inhalation URF (μg/m³)$^{-1}$		C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$		C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	162.18
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	284.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	1.10E-04 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	1.50E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.19E-05
D_a (cm²/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.06E-02
D_w (cm²/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	7.16E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	4.57E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.68E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.68E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.26E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.73E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999995
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.23E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.92E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.12E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.12E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.20E+00
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.20E+00

CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.63E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.15E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.39E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.63E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	9.06E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.19E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1995b)	C-1-7	1.80E-01
RfC (mg/m³)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from *Oral CSF* using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	5.10E-05
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	1.80E-01

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-172

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	78.96
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	490.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.03E-01
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.20E-05
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)		--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
ksg (year)⁻¹	--	B-1-2; B-2-2; B-3-2; B-4-2	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
	Biotransfer Factors for Plants		
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	--	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	2.20E-02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value for fruits was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1993e) for garden fruits. Br_{ag} value for vegetables was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2×10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1993e). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	1.95E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-8	1.60E-02
Br_{grain} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{grain} value was calculated by multiplying the uptake slope factors with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals.	B-3-8	2.00E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 87% moisture content in milk.	B-3-11	5.86E-03
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in beef.	B-3-10	2.27E-03
Ba_{pork} (day/kg FW)	Ba_{pork} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 4.7 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in pork.	B-3-12	1.88E-01
Ba_{egg} (day/kg FW)	Ba_{egg} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in eggs.	B-3-13	1.13E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in chicken.	B-3-14	1.13E+00
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	1.29E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	5.0E-03
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.8E-02
Inhalation URF (μg/m³)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-173

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	107.87
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	1,233.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.38E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	9.71E-06
K_{aw} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
ksg (year)$^{-1}$	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	--	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{root\ veg}$.	B-2-10	1.00E-01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	1.38E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Bv values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{forage}.	B-3-8	4.00E-01
Br_{grain} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{grain} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{grain}.	B-3-8	1.00E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed not to experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	2.0E-02
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	3.0E-03
Ba_{pork} (day/kg FW)	NC DEHNR (1997)	B-3-12	ND
Ba_{egg} (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	2.04E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-03
$Oral\ CSF$ $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.80E-02
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-174

CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	334.40
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	541.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	2.20E-13 at 25°C (solid)
S (mg/L)	Montgomery and Welkom (1991)	--	1.50E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.90E-13
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.38E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.58E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	8.51E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.53E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.53E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.40E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.81E+00

CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.085669
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis using a moisture content of 87 percent.	B-2-10	1.34E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kds value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	2.96E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.97E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.97E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vight (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.29E+07
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vight (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.29E+07

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.76E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.14E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	2.59E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.76E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	1.69E-06
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.72E+01
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-04
Oral CSF (mg/kg/day)$^{-1}$	—	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70kg.	C-2-3	1.1E-03
Inhalation URF (μg/m^3)$^{-1}$	—	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	—	C-2-2	ND

Note:

NA = Note applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
**Chemical/Physical Properties**			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	104.14
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	242.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	8.21E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.57E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.33E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.73E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.77E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	8.49E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	9.12E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.12E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.84E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.65E+01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \; DW \; plant}{\mu g/mL \; soil \; water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.81E+01
$Br_{root\,veg}$ $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{root\,veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.28E+00
Br_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	7.85E-01
Br_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	7.85E-01
Bv_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.21E-02
Bv_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.21E-02

CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.74E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.13E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.58E-05
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.74E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.68E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	9.91E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-01
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	1.0E+00
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)DIOXIN (1746-01-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	--	321.98
T_m (K)	U.S. EPA (1994a)	--	578.1
Vp (atm)	U.S. EPA (1994a)	--	4.45E-11 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	4.83E-04
H (atm·m³/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.60E-05
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.27E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.81E-06
K_{ow} (unitless)	U.S. EPA (1994a)	--	4.37E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994b). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.69E+04
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.69E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.02E+05
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.08E+05

TABLE A-3-176

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)DIOXIN (1746-01-6)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	4.29E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.977776
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g \; DW \; plant}{\mu g/mL \; soil \; water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.01E+04
$Br_{root \; veg}$ $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	$Br_{root \; veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.12E+00
Br_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.62E-03
Br_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.62E-03
Bv_{ag} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	6.10E+04
Bv_{forage} $(\dfrac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	6.10E+04

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)DIOXIN (1746-01-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	5.42E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chickens}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	7.30E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	1.00
Health Benchmarks			
RfD (mg/kg/day)		C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997c)	C-1-7	1.5E+05
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	U.S.EPA (1997c)	C-2-1	3.3E-08
Inhalation CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997c)	C-2-2	1.5E+05

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-177

CHEMICAL-SPECIFIC INPUTS FOR
2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	305.98
T_m (K)	U.S. EPA (1994a)	--	500.1
Vp (atm)	U.S. EPA (1994a)	--	1.97E-11 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	4.19E-04
H (atm·m³/mol)	U.S. EPA (1994a).	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.60E-06
D_a (cm²/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.79E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.85E-06
K_{ow} (unitless)	U.S. EPA (1992d)	--	3.39E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.09E+06
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.09E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.57E+05

**CHEMICAL-SPECIFIC INPUTS FOR
2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)**

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.36E+04
ksg (year)⁻¹	ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.767641
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.48E+04
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.19E+00
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.51E-03
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.51E-03
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	8.10E+04
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	8.10E+04

**CHEMICAL-SPECIFIC INPUTS FOR
2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)**

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	3.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	1.63E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	1.97E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	3.61E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	5.63E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.10
Health Benchmarks			
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ ($\mu g/m^3$)$^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

NA = Not Applicable
ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	215.89
T_m (K)	Montgomery and Welkom (1991)	--	411.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	7.1E-06 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	1.30E+00
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.18E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.11E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.75E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	4.36E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.89E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.89E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.42E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.36E+02

TABLE A-3-178

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999994
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.75E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.49E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.06E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.06E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.14E+00
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.14E+00

TABLE A-3-178

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.47E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.10E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.33E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.47E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	8.66E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.30E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-04
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.1E-03
Inhalation URF (μg/m³)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-179

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	167.85
T_m (K)	Montgomery and Welkom (1991)	--	230.1
Vp (atm)	Vp value cited in U.S. EPA (1995b)	--	1.60E-02 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b)	--	1.10E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.44E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.15E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.30E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	4.27E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.59E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.59E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.20E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.37E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	5.75E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}\right)$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.09E+01
$Br_{rootveg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.94E+01
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.17E+00
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.17E+00
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.45E-02
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.45E-02

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.39E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.07E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.30E-05
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.39E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	8.46E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.87E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	2.6E-02
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E-01
$Inhalation\ URF$ (μg/m^3)$^{-1}$	U.S. EPA (1997b)	C-2-1	7.4E-06
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	2.6E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	167.86
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	229.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	6.80E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.07E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.72E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.16E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.26E-06
K_{sw} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	4.40E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	7.90E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.90E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.93E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.16E+00

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	5.75E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.80E+02
$Br_{root \ veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.11E+03
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.02E-02
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.02E-02
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.33E+01
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.33E+01

TABLE A-3-180

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.50E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.105E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.34E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.50E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	8.73E-04
BCF_{fish} (L/kg FW tissue)	---	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.33E+03
$BSAF_{fish}$ (unitless)	---	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	---	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	2.0E-01
RfC (mg/m³)	---	C-2-3	ND
Inhalation URF (µg/m³)$^{-1}$	U.S. EPA (1997b)	C-2-1	5.8E-05
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	2.0E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	165.85
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	251.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	2.42E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	2.32E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.73E-02
D_a (cm²/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.20E-02
D_w (cm²/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	8.20E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	3.51E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.65E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.65E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.99E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.06E+01

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.75E+01
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.04E-03
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.31E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.31E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.66E-03
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.66E-03

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.79E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.82E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.07E-05
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.79E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	6.96E-06
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.06E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997e)	C-1-7	5.2E-02
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.5E-02
Inhalation URF $(\mu g/m^3)^{-1}$	U.S.EPA (1997e)	C-2-1	5.8E-07
Inhalation CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997e)	C-2-2	2.0E-03

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1995b)	--	231.89
T_m (K)	U.S. EPA (1995b)	--	343.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	6.60E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.00E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from, Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.53E-05
D_a (cm²/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.55E-02
D_w (cm²/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	5.78E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.0E+04
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH K_{oc} 1 6,190 2 6,188 3 6,166 4 5,956 5 4,456 6 1,323 7 249.2 8 115.3 9 101.6 10 100.2 11 100.0 12 100.0 13 100.0 14 100.0
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.49
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	18.69

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	9.97
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999968
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.83E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kds value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	1.94E+02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.27E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.27E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-9	1.39E+02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.39E+02

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.59E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.02E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	6.08E-04
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.59E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	3.97E-04
BCF_{fish} (L/kg, FW tissue)	—	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.63E+03
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-02
$Oral\ CSF$ $(mg/kg/day)^{-1}$	—	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.1E-01
$Inhalation\ URF$ $(\mu g/m^3)^{-1}$	—	C-2-1	ND
$Inhalation\ CSF$ $(mg/kg/day)^{-1}$	—	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	72.1
T_m (K)	Montgomery and Welkom (1991)	--	164.6
Vp (atm)	Vp value cited in Budavari, O'Neil, Smith, and Heckleman (1989).	--	2.14E-01 at 25°C (liquid)
S (mg/L)		--	ND
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.31E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.07E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994g).	--	2.80E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.16E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.16E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.37E-01

TABLE A-3-183

CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.26E-01
ksg (year)⁻¹	ksg value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	4.43E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.82E+00
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.16E+02
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.14E+01
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.14E+01
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	--	B-2-8	ND
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	--	B-3-8	ND

CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.22E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.03E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	8.51E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.22E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.55E-08
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.29E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m³)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-184

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	204.38
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	576.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.48E-02
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	6.34E-06
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
ksg (year)⁻¹	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000
Biotransfer Factors for Plants			
RCF $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}\right)$	---	B-2-10	ND
$Br_{rootveg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{root\,veg}$.	B-2-10	4.00E-04
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative (reproductive) growth and Bv values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	8.58E-04
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Bv values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{forage}.	B-3-8	4.00E-03
Br_{grain} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{grain} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). Br values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{grain}.	B-3-8	4.00E-04
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

TABLE A-3-184

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	2.0E-03
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	4.0E-02
Ba_{pork} (day/kg FW)	--	B-3-12	ND
Ba_{egg} (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	1.40E+03
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	8.0E-05
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.8E-04
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	92.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	3.71E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	5.58E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.13E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.72E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	4.65E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.40E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.05E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.60E+00

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.15E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.26E+01
$Br_{root\,veg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{root\,veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.33E+01
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.11E+00
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.11E+00
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.33E-03
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.33E-03

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.69E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.17E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.41E-05
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.69E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	9.22E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.27E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	4.0E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	107.15
T_m (K)	Montgomery and Welkom (1991)	--	258.4
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	3.94E-04 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	1.74E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.43E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.14E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.12E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	2.19E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.57E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.57E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.18E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.28E-01

CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999998
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.81E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	5.61E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.51E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.51E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.16E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.16E-01

CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.74E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.50E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	6.65E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.74E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.34E-07
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.14E+00
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	—	C-1-8	NA
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1995b)	C-1-7	2.4E-01
RfC (mg/m^3)	—	C-2-3	NA
$Inhalation\ URF$ (μg/m^3)$^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	6.9E-02
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	Value beased on Oral CSF assuming route-to-route extrapolation.	C-2-2	2.4E-01

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	181.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	325.7
Vp (atm)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	--	3.20E-04 at 25°C (solid)
S (mg/L)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	--	2.05E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.84E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.02E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.15E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.11E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.02E+04
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.02E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.52E+03
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.10E+02

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999999
Biotransfer Factors for Plants			
RCF $(\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	3.09E+02
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.53E+00
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.78E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.78E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	4.01E-01
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	4.01E-01

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	8.82E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.79E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.38E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	8.82E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.20E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with an estimated BCF. $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	8.76E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-188

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	181.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	290.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	4.42E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	3.07E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.61E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.00E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	9.73E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.66E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.66E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.24E+02
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table. .	B-4-16; B-4-25	6.64E+01

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999999
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.80E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.69E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.92E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.92E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.78E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.78E-01

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.73E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.45E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.96E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.73E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.93E-04
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.33E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997c)	C-2-3	2.0E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	133.42
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	242.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	1.63E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.17E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.86E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.64E+02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.56E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	2.64E+02
K_{oc} (mL/g)	Geometric mean value cited in U.S. EPA (1996b)	--	1.35E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.35E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.01E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.40E+00
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.27E-01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7;	1.000000

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF ($\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$)	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	2.33E+01
$Br_{root\ veg}$ ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.73E+01
Br_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.54E+00
Br_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.54E+00
Bv_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.14E-03
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.14-03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.10E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.63E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	8.03E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.10E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value:	B-3-14	5.24E-06

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.08E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	3.50E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	NA
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.23E-01
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	133.42
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	238.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	3.31E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	4.40E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.00E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.51E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.0E-05
K_{sw} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.25E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	7.50E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.50E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.63E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.00E+00

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	6.93E-01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.59E+01
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.12E+01
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.38E+00
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.38E+00
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	9.53E-03
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	9.53E-03

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.93E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.14E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	3.80E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.93E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	2.48E-06
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.31E+01
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	4.0E-03
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	C-1-7	5.70E-02
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.4E-02
$Inhalation\ URF$ (μg/m³)$^{-1}$	U.S. EPA (1997b)	C-2-1	1.6E-05
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	5.7E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	131.40
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	188.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	9.48E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.18E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.06E-02
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.65E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.94E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.71E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.40E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.40E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.05E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.76E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	0.703
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.37E+01
$Br_{root \ veg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.12E+01
Br_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.52E+00
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.52E+00
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.07E-03
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.07E-03

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.15E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.81E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	8.24E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.15E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	5.37E-06
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.16E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997a)	C-1-8	6.0E-03
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1995b)	C-1-7	1.1E-02
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.1E-02
$Inhalation\ URF$ (μg/m^3)$^{-1}$	U.S. EPA (1995b)	C-2-1	1.7E-06
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	1.1E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

<u>**(Page 1 of 3)**</u>

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	137.38
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	162.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	1.10E+00 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	1.10E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.37E-01
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.27E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.0E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	--	3.40E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.34E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.34E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.00E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs} because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.34E+00

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.70E+01
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.02E+00
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.33E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.33E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.02E-04
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.02E-04

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.70E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.54E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.03E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.70E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	6.74E-06
BCF_{fish} (L/kg, FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.94E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-01
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997c)	C-2-3	7.0E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	197.46
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	340.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.15E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.53E+02
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.64E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.91E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.03E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	7.41E+03
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH K_{oc} 1 2,380 2 2,380 3 2,380 4 2,377 5 2,353 6 2,139 7 1,127 8 223.7 9 56.14 10 37.94 11 36.10 12 35.92 13 35.90 14 35.90
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.13E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	8.45E+01

TABLE A-3-193

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	4.51E+01
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	0.367
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999989
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.28E+02
$Br_{root\,veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\,veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.02E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.24E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.24E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.31E+02
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.31E+02

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.89E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.86E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.25E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.89E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.47E-04
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.14E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-01
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.5E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	197.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	342.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.55E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.53E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.06E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.62E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.08E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.15E+03
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH K_{oc} 1 1,070 2 1,070 3 1,069 4 1,063 5 1,006 6 670.8 7 226.2 8 120.4 9 108.4 10 107.1 11 107.0 12 107.0 13 107.0 14 107.0
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.26E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	1.70E+01

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	9.05E+00
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.61E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999986
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.74E+02
$Br_{root\ veg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	7.69E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.77E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.77E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.23E+02
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.23E+02

TABLE A-3-194

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.09E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.29E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.57E-04
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.09E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.02E-04
BCF_{fish} (L/kg, FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.90E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	--
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1995b)	C-1-7	1.1E-02
RfC (mg/m^3)	--	C-2-3	--
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997)	C-2-1	3.1E-06
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	--

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	--	147.43
T_m (K)	Montgomery and Welkom (1991)	--	258.4
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	4.90E-03 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	1.90E+03
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.80E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.99E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.24E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.78E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	8.05E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.10E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.04E+00
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.22E+00

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.89E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.34E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.94E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.94E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	3.66E-02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.66E-02

TABLE A-3-195

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.41E-06
Ba_{beef} (day/kg FW	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.47E-06
Ba_{pork} (day/kg FW	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	5.41E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.41E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.53E-06
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.02E+01
BAF_{fish} (L/kg FW	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	6.0E-03
$Oral\ CSF$ (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-1-7	7.0E+00
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.1E-02
$Inhalation\ URF$ ($\mu g/m^3$)$^{-1}$	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	2.0E-03
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	7.0E+00

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	120.19
T_m (K)	Montgomery and Welkom (1991)	--	287.9
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	1.30E-03 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1992a).	--	2.00E+01
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.81E-03
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.48E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.86E-06
K_{ow} (unitless)	K_{ow} value cited in Howard (1989-1993).	--	2.63E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.67E+03
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.67E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.25E+02

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.69E+01
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	3.16E+01
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.06E+02
$Br_{root \ veg}$ $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	6.35E+00
Br_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.09E-01
Br_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.09E-01
Bv_{ag} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.14E-02
Bv_{forage} $(\dfrac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.14E-02

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.09E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.61E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	8.00E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.09E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.22E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.34E+02
BAF_{fish} (L/kg FW)	—	B-4-27	NA
$BSAF_{fish}$ (unitless)	—	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	5.0E-02
$Oral\ CSF$ (mg/kg/day)$^{-1}$		C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.8E-01
$Inhalation\ URF$ (μg/m^3)$^{-1}$		C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$		C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-197

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	213.11
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	395.6
Vp (atm)	Vp value cited in U.S. EPA (1995b).	--	1.30E-07 at 25°C (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).	--	3.20E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.66E-08
D_a (cm²/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.84E-02
D_w (cm²/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	6.08E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.51E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.18E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.18E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.84E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.72E-01

A-3-661

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999504
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.19E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	6.95E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.05E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.05E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.17E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.17E+01

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.20E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.80E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.60E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.20E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.00E-07
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.64E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-02
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-198

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	227.13
T_m (K)	Montgomery and Welkom (1991)	--	353.2
Vp (atm)	--	--	ND
S (mg/L)	--	--	ND
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.62E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.85E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	3.98E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.51E+01
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.51E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw} because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.88E+00

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.00E+00
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
Fv (unitless)	Fv value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.03E+01
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	4.10E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.60E+00
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.60E+00
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	--	B-2-8	ND
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	--	B-3-8	ND

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.16E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.00E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.21E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.16E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	7.89E-07
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	9.68E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	3.0E-02
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.8E-03
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from Oral CSF using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-1	8.6E-06
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-2-2	3.0E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	86.09
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	180.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.43E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.24E+04
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.50E-04
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.94E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.00E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.00E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.97E+00
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.97E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.73E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.99E-01

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.11E+00
$Br_{root\ veg}$ $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	1.43E+02
Br_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.53E+01
Br_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil}\right)$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.53E+01
Bv_{ag} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	5.65E-04
Bv_{forage} $\left(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air}\right)$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	5.65E-04

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.97E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.26E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.52E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.97E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	9.92E-08
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.00E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	1.0E+00
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	2.0E-01
Inhalation URF (μg/m^3)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	62.50
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	119.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	3.68E+00 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.30E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.15E-01
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.58E-01
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.19E-05
K_{sw} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.40E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.11E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.11E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.32E-01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.44E-01
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.000000
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.08E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	7.29E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.42E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.42E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci and others (1990; 1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	2.95E-06
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	2.95E-06

CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.11E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.52E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	4.26E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.11E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-14	2.78E-07
BCF_{fish} (L/kg, FW tissue)	$BAFs$ were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). BAF values were predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-26	4.37E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-1-7	1.9E+00
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF (μg/m^3)$^{-1}$	U.S. EPA (1997c)	C-2-1	8.4E-05
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	C-2-2	3.0E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-201

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.16
T_m (K)	Montgomery and Welkom (1991)	--	225.7
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	1.39E-05 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1992a).	--	1.60E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.26E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.69E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.49E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	1.59E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.96E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.96E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.47E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	7.84E+00
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7;	0.999957

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

(Page 2 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	7.41E+01
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	3.78E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.47E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.47E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.55E+01
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.55E+01

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.26E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.99E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.83E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.26E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.15E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.60E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.0E+00
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	7.0E+00
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-202

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.16
T_m (K)	Montgomery and Welkom (1991)	--	248.1
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	1.39E-05 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1992a).	--	2.20E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.73E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.69E-02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.44E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	1.35E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.41E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.41E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.81E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	9.64E+00
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7;	0.999957

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\dfrac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	6.61E+01
$Br_{rootveg}$ $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.74E+01
Br_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.01E-01
Br_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.01E-01
Bv_{ag} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.79E+01
Bv_{forage} $(\dfrac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.79E+01

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.07E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.39E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.10E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.07E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.68E-05
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.41E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.0E+00
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	7.0E+00
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
	Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.16
T_m (K)	Montgomery and Welkom (1991)	--	286.1
Vp (atm)	Vp value cited in U.S. EPA (1992a).	--	1.39E-05 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1992a).	--	2.15E+02
H (atm·m³/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.89E-06
D_a (cm²/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.61E+02
D_w (cm²/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.50E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	1.48E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	3.11E+02
Kd_s (cm³/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.11E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.33E+01
Kd_{bs} (cm³/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.24E+01
ksg (year)⁻¹	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.03E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7;	0.999957

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \; WW \; plant}{\mu g/mL \; soil \; water}$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-10	7.05E+01
$Br_{rootveg}$ $(\frac{\mu g/g \; WW \; plant}{\mu g/g \; soil})$	$Br_{rootveg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.27E+01
Br_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.70E-01
Br_{forage} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.70E-01
Bv_{ag} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.93E+01
Bv_{forage} $(\frac{\mu g/g \; DW \; plant}{\mu g/g \; air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.93E+01

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.18E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.72E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.50E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.18E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.93E-05
BCF_{fish} (L/kg FW tissue)	$BCFs$ were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.51E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.0E+00
$Oral\ CSF$ (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from RfD using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E+00
$Inhalation\ URF$ (μg/m^3)$^{-1}$	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-204

CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

(Page 1 of 3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	65.38
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	692.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water. OR Budavari, O'Neil, Smith, and Heckelman (1989)	--	0.0
H (atm·m³/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm²/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.17E-01
D_w (cm²/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.36E-05
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.2E+01 at pH=6.8
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	6.2E+01 at pH=6.8
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	6.2E+01 at pH=6.8
ksg (year)⁻¹	--	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.000000

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $\frac{\mu g/g \ DW \ plant}{\mu g/mL \ soil \ water}$	--	--	ND
$Br_{rootveg}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{rootveg}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	4.40E-02
$Br_{ag \ (fruit)}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg.}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for garden fruits.	B-2-9	4.60E-02
$Br_{ag \ (veg)}$ $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg}$ value was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2×10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1992b).	B-3-9	9.70E-02
Br_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg.}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-9	2.50E-01
Br_{grain} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ soil})$	$Br_{root \ veg.}$ value was calculated by multiplying the uptake slope factors with a conversion factor of 2×10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals.	B-3-9	5.40E-02
Bv_{ag} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $(\frac{\mu g/g \ DW \ plant}{\mu g/g \ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 87% moisture content in milk.	B-3-11	3.25E-05

CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

(Page 3 of 3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals (Continued)			
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in beef.	B-3-10	9.00E-05
Ba_{pork} (day/kg FW)	Ba_{pork} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 4.7 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in pork.	B-3-12	1.28E-04
Ba_{egg} (day/kg FW)	Ba_{egg} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in eggs.	B-3-13	8.75E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in chicken.	B-3-14	8.75E-03
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4.).	B-4-26	6.54E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-01
Oral CSF (mg/kg/day)$^{-1}$	--	C-1-7	ND
RfC (mg/m³)	Calculated from RfD using an inhalation rate of 20 m³/day and a human body weight of 70 kg.	C-2-3	1.1E+00
Inhalation URF (μg/m³)$^{-1}$	--	C-2-1	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable;
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

APPENDIX A-4

ACUTE INHALATION EXPOSURE CRITERIA

TABLE A-4

ACUTE INHALATION EXPOSURE CRITERIA

(Page 1 of 6)

Compound	CAS Number	AEGL-1 (mg/m³)	ERPG-1 (mg/m³)	ATEL-1 (mg/m³)	TEEL-1 (mg/m³)
Acetophenone	98-86-2	--	--	--	3.01E+01
Acrolein	107-02-8	--	2.29E-01	1.17E-04	2.29E-01[a]
Acrylonitrile	107-13-1	--	2.17E+01	--	2.17E+01[a]
Aniline	62-53-3	3.05E+01	--	--	5.98E+00
Anthracene	120-12-7	--	--	--	--
Benzene	71-43-2	--	1.60E+02	7.67E-01	1.60E+02[a]
Benzo(a)anthracene	56-55-3	--	--	--	--
Benzo(a)pyrene	50-32-8	--	--	--	1.00E+00
Benzo(b)fluoranthene	205-99-2	--	--	--	--
Benzo(k)fluoranthene	207-08-9	--	--	--	--
Benzyl Chloride	100-44-7	--	5.18E+00	1.55E-01	5.18E+00[a]
Bromodichloromethane	75-27-4	--	--	--	--
Bromoform	75-25-2	--	--	--	1.55E+01
Bromomethane (Methyl bromide)	74-83-9	--	--	--	5.83E+01
Butanone, 2- (Methyl Ethyl Ketone)	78-93-3	--	--	5.90E-02	8.85E+02
Butylbenzyl Phthalate	85-68-7	--	--	--	--
Carbon Tetrachloride	56-23-5	--	1.26E+02	8.18E-01	1.26E+02[a]
Carbon Disulfide	75-15-0	--	3.11E+00	--	3.74E+01
Chlordane	57-74-9	--	--	--	1.49E+00
Chloroaniline, p-	106-47-8	--	--	--	3.00E+01
Chlorobenzene	108-90-7	--	--	--	3.45E+02

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TABLE A-4

ACUTE INHALATION EXPOSURE CRITERIA

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Compound	CAS Number	AEGL-1 (mg/m³)	ERPG-1 (mg/m³)	ATEL-1 (mg/m³)	TEEL-1 (mg/m³)
Chlorobenzilate	510-15-6	--	--	--	--
Chloroethyl ether, 2-bis	111-44-4	--	--	--	5.85E+01
Chloroform (Trichloromethane)	67-66-3	--	--	3.56E-01	4.88E+02
Chloromethane (Methyl chloride)	74-87-3	--	-	--	2.07E+02
Chloronaphthalene, 2-	91-58-7	--	--	--	5.99E-01
Chlorophenol, 2-	95-57-8	--	--	--	6.31E+00
Chrysene	218-01-9	--	--	--	2.99E-01
Cresol, p-	106-44-5	--	--	--	6.63E+01[b]
Cresol, o-	95-48-7	--	--	--	6.63E+01[b]
Cresol, m-	108-39-4	--	--	--	6.63E+01[b]
DDE	72-55-9	--	--	--	3.00E+01
Dibenzo(a,h)anthracene	53-70-3	--	--	--	3.01E+01
Dibromo-3-Chloropropane, 1,2-	96-12-8	--	--	--	--
Dibutyl Phthalate	84-74-2	--	--	--	1.50E+01
Dichlorobenzene, 1,2-	95-50-1	--	--	--	3.01E+02
Dichlorobenzene, 1,4-	106-46-7	--	--	--	6.61E+02
Dichlorobenzidine, 3,3'-	91-94-1	--	--	--	6.21E+00
Dichlorodifluoromethane	75-71-8	--	--	--	1.48E+04
Dichloroethane (Ethylene Dichloride), 1,2-	107-06-2	--	--	--	8.09E+00
Dichloroethane, 1,1-	75-34-3	--	--	--	1.21E+03
Dichloroethene, 1,2-(trans)	540-59-0	--	--	--	2.38E+03

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ACUTE INHALATION EXPOSURE CRITERIA

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Compound	CAS Number	AEGL-1 (mg/m³)	ERPG-1 (mg/m³)	ATEL-1 (mg/m³)	TEEL-1 (mg/m³)
Dichloroethene, 1,1-	75-35-4	--	--	--	7.93E+01
Dichlorophenol, 2,4-	120-83-2	--	--	--	3.00E+01
Dichloropropane, 1,2-	78-87-5	--	--	--	5.08E+02
Dichloropropene, 1,3-(cis)	542-75-6	--	--	--	1.36E+01
Diethyl Phthalate	84-66-2	--	--	--	1.50E+01
Dimethoxybenzidine, 3,3'-	119-90-4	--	--	--	5.00E+00
Dinitrobenzene, 1,3-	99-65-0	--	--	--	--
Dinitrophenol, 2,4-	51-28-5	--	--	--	9.79E-01
Dinitrotoluene, 2,4-	121-14-2	--	--	--	4.47E-01
Dinitrotoluene, 2,6-	606-20-2	--	--	--	4.47E-01
Dioxane (1,4-Diethyleneoxide), 1,4-	123-91-1	--	--	1.80E+00	2.70E+02
Diphenylhydrazine, 1,2-	122-66-7	--	--	--	3.00E+01
Epichlorohydrin (1-Chloro-2,3-epoxypropane)	106-89-8	--	7.57E+00	7.95E-01	7.57E+00[a]
Ethyl Methacrylate	97-63-2	--	--	--	--
Ethyl Methanesulfonate	62-50-0	--	--	--	--
Ethyl Benzene	100-41-4	--	--	--	5.43E+02
Ethylene Oxide	75-21-8	--	--	--	9.01E+00
Ethylene Dibromide	106-93-4	--	--	--	2.31E+02
Fluoranthene	206-44-0	--	--	--	--
Heptachlor	76-44-8	--	--	--	1.50E-01
Hexachlorobenzene (Perchlorobenzene)	118-74-1	--	--	--	7.45E-02

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ACUTE INHALATION EXPOSURE CRITERIA

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Compound	CAS Number	AEGL-1 (mg/m³)	ERPG-1 (mg/m³)	ATEL-1 (mg/m³)	TEEL-1 (mg/m³)
Hexachlorobutadiene (Perchlorobutadiene)	87-68-3	--	3.20E+01	--	3.20E+01[a]
Hexachlorocyclopentadiene	77-47-4	--	--	--	2.23E-01
Hexachloroethane (Perchloroethane)	67-72-1	--	--	--	2.90E+01
Hexachlorophene	70-30-4	--	--	--	3.00E+01
Indeno(1,2,3-cd)pyrene	193-39-5	--	--	--	--
Methoxychlor	72-43-5	--	--	--	--
Methyl Isobutyl Ketone	108-10-1	--	--	--	3.07E+02
Methylene Chloride	75-09-2	--	6.95E+02	8.16E+01	6.95E+02[a]
N-Nitroso di-n-Butylamine	924-16-3	--	--	--	--
Naphthalene	91-20-3	--	--	--	7.86E+01
Nitrobenzene	98-95-3	--	--	--	1.51E+01
Pentachlorobenzene	608-93-5	--	--	--	1.00E+00
Pentachloronitrobenzene	82-68-8	--	--	--	1.45E+00
Pentachlorophenol	87-86-5	--	--	--	1.53E+00
Phenol	108-95-2	--	3.85E+01	--	3.85E+01[a]
Phthalic Anhydride (1,2-Benzenedicarboxylic Anhydride)	85-44-9	--	--	--	1.80E+01
Pyridine	110-86-1	--	--	--	4.85E+01
Safrole (5-(2-Propenyl)-1,3-Benzodioxole)	94-59-7	--	--	--	--
Strychnine	57-24-9	--	--	--	3.01E-01
Styrene	100-42-5	--	2.13E+02	2.16E+01	2.13E+02[a]
Tetrachlorethane, 1,1,1,2-	630-20-6	--	--	--	6.18E+01

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ACUTE INHALATION EXPOSURE CRITERIA

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Compound	CAS Number	AEGL-1 (mg/m³)	ERPG-1 (mg/m³)	ATEL-1 (mg/m³)	TEEL-1 (mg/m³)
Tetrachlorobenzene, 1,2,4,5-	95-94-3	--	--	--	3.00E+01
Tetrachlorodibenzo(p) dioxin, 2,3,7,8-	1746-01-6	--	--	--	--
Tetrachloroethane, 1,1,2,2-	79-34-5	--	--	--	2.06E+01
Tetrachloroethene	127-18-4	--	6.78E+02	--	6.78E+02[a]
Tetrachlorophenol, 2,3,4,6-	58-90-2	--	--	--	--
Toluene	108-88-3	--	1.88E+02	3.66E+01	1.88E+02[a]
Toluidine, o-	95-53-4	--	--	--	2.63E+01
Trichlorobenzene, 1,2,4-	120-82-1	--	--	--	2.23E+01
Trichloroethane, 1,1,2-	79-00-5	--	--	--	1.64E+02
Trichloroethylene	79-01-6	--	5.37E+02	--	5.37E+02[a]
Trichlorofluoromethane (Freon 11)	75-69-4	--	--	--	2.81E+03
Trichlorophenol, 2,4,5-	95-95-4	--	--	--	2.99E+01
Trichlorophenol, 2,4,6-	88-06-2	--	--	--	3.00E+01
Trichloropropane, 1,2,3-	96-18-4	--	--	--	--
Trinitrobenzene, 1,3,5-	99-35-4	--	--	--	3.00E+01
Vinyl Acetate	108-05-4	--	1.76E+01	--	1.76E+01[a]
Vinyl Chloride	75-01-04	--	--	2.07E+02	1.28E+01
Antimony	7440-36-0	--	--	--	1.49E+00
Arsenic	7440-38-2	--	--	--	3.00E-02
Barium	7440-39-3	--	--	--	1.52E+00
Beryllium	7440-41-7	--	--	--	9.95E-03

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Compound	CAS Number	AEGL-1 (mg/m³)	ERPG-1 (mg/m³)	ATEL-1 (mg/m³)	TEEL-1 (mg/m³)
Cadmium	7440-43-9	--	--	--	**2.99E-02**
Chromium (Total)	7440-47-3	--	--	--	**1.49E+00**
Chromium (hexavalent)	18540-29-9	--	--	--	**1.50E-01**
Lead	7439-92-1	--	--	--	**3.81E-02**
Mercury	7439-97-6	--	--	--	**7.38E-02**
Nickel	7440-02-0	--	--	**1.56E-03**	3.00E+00
Selenium	7782-49-2	--	--	**2.94E-03**	5.81E-01
Silver	7440-22-4	--	--	--	**3.00E-01**
Thallium	7440-28-0	--	--	--	**1.34E-01**

Notes:

Bolded values are the U.S. EPA OSW recommended AIECvalues for a few potential COPCs.

mg/m³	=	milligrams per cubic meter
--	=	AIEC value not available
CAS	=	Chemical abstract service
AEGL-1	=	Level 1 Acute Exposure Guideline Levels for 1-hour exposure durations (NAC 1997)
ERPG-1	=	Level 1 Emergency Response Planning Guideline Levels (SCAPA 1997b)
ATEL-1	=	Level 1 Acute Toxic Exposure Levels (Cal/EPA 1995)
TEEL-1	=	Level 1 Temporary Emergency Exposure Limits (SCAPA 1997a)
a	=	TEEL-1 value is based on ERPG-1 value
b	=	Equals TEEL-1 value for sum of all three cresol isomers.

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